

# Optimal bounds for aggregation of affine estimators

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## Abstract

We study the problem of aggregation of estimators when the estimators are not independent of the data used for aggregation and no sample splitting is allowed. If the estimators are deterministic vectors, it is well known that the minimax rate of aggregation is of order  $\log(M)$ , where  $M$  is the number of estimators to aggregate. It is proved that for affine estimators, the minimax rate of aggregation is unchanged: it is possible to handle the linear dependence between the affine estimators and the data used for aggregation at no extra cost. The minimax rate is not impacted either by the variance of the affine estimators, or any other measure of their statistical complexity. The minimax rate is attained with a penalized procedure over the convex hull of the estimators, for a penalty that is inspired from the  $Q$ -aggregation procedure. The results follow from the interplay between the penalty, strong convexity and concentration.

## 1 Introduction

We study the problem of recovering an unknown vector  $\mathbf{f} = (f_1, \dots, f_n)^T \in \mathbf{R}^n$  from noisy observations

$$Y_i = f_i + \xi_i, \quad i = 1, \dots, n, \quad (1.1)$$

where the noise random variables  $\xi_1, \dots, \xi_n$  are i.i.d.  $\mathcal{N}(0, \sigma^2)$  or i.i.d. sub-gaussian random variables. We measure the quality of estimation of the unknown vector  $\mathbf{f}$  with the squared Euclidean norm in  $\mathbf{R}^n$ :

$$\|\mathbf{f} - \hat{\boldsymbol{\mu}}\|_2^2,$$

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for any estimator  $\hat{\boldsymbol{\mu}}$  of  $\mathbf{f}$ . When the noise random variables are normal, (1.1) is the Gaussian sequence model, which has been extensively studied, see e.g. [27] and the references therein. Several estimators have been proposed to recover the unknown vector  $\mathbf{f}$  from the observations: the Ordinary Least Squares, the Ridge estimator, the Stein estimator and the procedures based on shrinkage, to name a few. Several of these estimators depend on a parameter that must be chosen carefully to obtain satisfying error bounds. These available estimators have different strengths and weaknesses in different scenarios, so it is important to be able to mimic the best among a given family of estimators, without any assumption on the unknown  $\mathbf{f}$ . The problem of mimicking the best estimator in a given finite set is the problem of model-selection type aggregation, which was introduced in [34, 42]. More precisely, let  $\hat{\boldsymbol{\mu}}_1, \dots, \hat{\boldsymbol{\mu}}_M$  be  $M$  estimators of  $\mathbf{f}$  based on the data  $\mathbf{y} = (Y_1, \dots, Y_n)^T$ . The goal is to construct with the same data  $\mathbf{y} = (Y_1, \dots, Y_n)^T$  a new estimator  $\hat{\boldsymbol{\mu}}$  called the aggregate, which satisfies with probability greater than  $1 - \delta$  the sharp oracle inequality<sup>1</sup>

$$\|\hat{\boldsymbol{\mu}} - \mathbf{f}\|_2^2 \leq \min_{j=1, \dots, M} \|\hat{\boldsymbol{\mu}}_j - \mathbf{f}\|_2^2 + \text{PRICE}_M(\delta), \quad (1.2)$$

where  $\text{PRICE}_M(\cdot)$  is a function of  $\delta$  that should be small. The term  $\text{PRICE}_M(\cdot)$  will be referred to as the price to pay for aggregating the estimators  $\hat{\boldsymbol{\mu}}_1, \dots, \hat{\boldsymbol{\mu}}_M$ . If the estimators  $\hat{\boldsymbol{\mu}}_1, \dots, \hat{\boldsymbol{\mu}}_M$  are deterministic vectors, the price to pay for aggregating these estimators is of order  $\sigma^2 \log(M/\delta)$  and (1.2) is satisfied for an estimator  $\hat{\boldsymbol{\mu}}$  based on  $Q$ -aggregation [12]. Considering deterministic estimators is of interest if two independent samples are available, so that  $\hat{\boldsymbol{\mu}}_1, \dots, \hat{\boldsymbol{\mu}}_M$  are based on the first sample while aggregation is performed using the second sample. Then the first sample can be considered as frozen at the aggregation step (for more details see [41]). If the estimators are random (dependent on the data  $\mathbf{y}$  used for aggregation), two natural questions arise.

1. Does the price to pay for aggregation increase because of the dependence between  $\hat{\boldsymbol{\mu}}_1, \dots, \hat{\boldsymbol{\mu}}_M$  and the data  $\mathbf{y}$ , or is it still of order  $\sigma^2 \log(M/\delta)$ ? Is there an extra price to pay to handle the dependence?
2. A natural quantity that captures the statistical complexity of a given estimator  $\hat{\boldsymbol{\mu}}_j$  is the variance defined by  $\mathbb{E}\|\hat{\boldsymbol{\mu}}_j - \mathbb{E}\hat{\boldsymbol{\mu}}_j\|_2^2$ . When the estimators are deterministic, their variances are all zero. Now that the estimators are random, does the price to pay for aggregation depend on the statistical complexities of the estimators  $\hat{\boldsymbol{\mu}}_1, \dots, \hat{\boldsymbol{\mu}}_M$ , for example

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<sup>1</sup>By sharp, we mean that the constant in front of the term  $\min_{j=1, \dots, M} \|\hat{\boldsymbol{\mu}}_j - \mathbf{f}\|_2^2$  is 1.

through their variances? Is it harder to aggregate estimators with large statistical complexities?

The goal of this paper is to answer these questions for affine estimators.

Among the procedures available to estimate  $\mathbf{f}$ , several are linear in the observations  $Y_1, \dots, Y_n$ . It is the case for the Least Squares and the Ridge estimators, whereas the shrinkage estimators and the Stein estimator are non-linear functions of the observations. Examples of estimators that are linear or affine in the observations is given in [14, Section 1.2], [1] and references therein. An affine estimator is of the form  $\hat{\boldsymbol{\mu}}_j = A_j \mathbf{y} + \mathbf{b}_j$  for a deterministic matrix  $A_j$  of size  $n \times n$  and a deterministic vector  $\mathbf{b}_j \in \mathbf{R}^n$ . The linearity of the estimators  $\hat{\boldsymbol{\mu}}_1, \dots, \hat{\boldsymbol{\mu}}_M$  makes it possible to explicitly treat the dependence between the estimators  $\hat{\boldsymbol{\mu}}_1, \dots, \hat{\boldsymbol{\mu}}_M$  and the data  $\mathbf{y} = (Y_1, \dots, Y_n)^T$  used to aggregate them. Donoho et al. [17] proved that for orthosymmetric quadratically convex sets (which include all ellipsoids and hyperrectangles), the minimax risk among all linear estimators is within 25% of the minimax risk among all estimators.

The papers [31, 14, 13] derived different procedures that satisfy sharp oracle inequalities for the problem of aggregation of affine estimators when the noise random variables are Gaussian. Leung and Barron [31], Dalalyan and Salmon [14] proposed an estimator  $\hat{\boldsymbol{\mu}}^{EW}$  based on exponential weights, for which the following sharp oracle inequality holds in expectation:

$$\mathbb{E} \|\mathbf{f} - \hat{\boldsymbol{\mu}}^{EW}\|_2^2 \leq \min_{j=1, \dots, M} \mathbb{E} \|\hat{\boldsymbol{\mu}}_j - \mathbf{f}\|_2^2 + 8\sigma^2 \log M,$$

under the assumption that all  $A_j$  are orthoprojectors (orthogonal projection matrices, cf (1.4)), or under a strong commutativity assumption on the matrices  $A_j$ . The constant 8 can be reduced to 4 if all  $A_j$  are orthoprojectors. If the matrices  $A_j$  are not symmetric, [14] achieved a similar oracle inequality by symmetrizing the affine estimators before the aggregation step, which suggests that the symmetry assumption can be relaxed. Although the estimator  $\hat{\boldsymbol{\mu}}^{EW}$  achieves this inequality in expectation, it was shown in [2, 12] that it cannot achieve a similar result in deviation, with an unavoidable error term of order  $\sqrt{n}$ . In Dai et al. [13], a sharp oracle inequality in deviation is derived for an estimator  $\hat{\boldsymbol{\mu}}^Q$  based on  $Q$ -aggregation [36, 12]. Namely, [13] proves that if the matrices  $A_1, \dots, A_M$  are symmetric and positive semi-definite, the estimator  $\hat{\boldsymbol{\mu}}^Q$  satisfies with probability greater than  $1 - \delta$ :

$$\|\mathbf{f} - \hat{\boldsymbol{\mu}}^Q\|_2^2 \leq \min_{j=1, \dots, M} \left( \|\hat{\boldsymbol{\mu}}_j - \mathbf{f}\|_2^2 + 4\sigma^2 \text{Tr}(A_j) \right) + C\sigma^2 \log(M/\delta), \quad (1.3)$$

where the constant  $C$  is proportional to the largest operator norm of the matrices  $A_1, \dots, A_M$ . The term  $4\sigma^2 \text{Tr}(A_j)$  is intimately linked to the statistical

complexity of the estimator  $\hat{\boldsymbol{\mu}}_j = A_j \mathbf{y} + \mathbf{b}_j$ . For instance, the variance of  $\hat{\boldsymbol{\mu}}_j$  is  $\mathbb{E}\|\hat{\boldsymbol{\mu}}_j - \mathbb{E}\hat{\boldsymbol{\mu}}_j\|_2^2 = \sigma^2 \text{Tr}(A_j^T A_j)$ . If  $\hat{\boldsymbol{\mu}}_j$  is a Least Squares estimator,  $A_j$  is an orthoprojector, and the variance becomes  $\sigma^2 \text{Tr} A_j$ . Thus, the statistical complexity of the estimator  $\hat{\boldsymbol{\mu}}_j$  clearly appears in the remainder term of the oracle inequality (1.3) proved in [13]. Thus, one may think that the price to pay for aggregating affine estimators, i.e. the function  $\text{PRICE}_M(\delta)$  in (1.2), depends on the statistical complexity of the estimators to aggregate.

The bound (1.3) may lead to the conclusion that the price to pay for aggregation of affine estimators can be substantially larger than  $\sigma^2 \log(M/\delta)$  which is the price for aggregating deterministic vectors. Indeed, the extra term  $4\sigma^2 \text{Tr}(A_j)$  may be large in common situation where the trace of some matrices  $A_j$  is large. For example, if one aggregates the estimators  $\hat{\boldsymbol{\mu}}_1 = \lambda_1 \mathbf{y}, \dots, \hat{\boldsymbol{\mu}}_M = \lambda_M \mathbf{y}$ , for some positive real numbers  $\lambda_1, \dots, \lambda_M$ , then the remainder term  $4\sigma^2 \text{Tr}(A_j)$  in the above oracle inequality is of order  $\sigma^2 n \lambda_j$  for each  $j = 1, \dots, M$ , which can be greater than the optimal rate  $\sigma^2 \log M$ . This term  $4\sigma^2 \text{Tr}(A_j)$  makes the oracle inequality (1.3) suitable only for scenarios where the matrices  $A_j$  have small trace. But more importantly, the term  $\sigma^2 \text{Tr} A_j$  suggests that the price to pay for aggregating affine estimators increases with the statistical complexities of the estimators to aggregate.

The results discussed above rely on specific assumptions on the matrices  $A_1, \dots, A_M$  [31, 14, 13]. This raises a third question, although not as important as the two questions above:

3. Does the nature of the matrices  $A_1, \dots, A_M$  have an impact on the price to pay to aggregate these affine estimators? Is the price in (1.2) substantially smaller if the matrices are orthoprojectors, semi-positive definite or symmetric?

The main contribution of the present paper is to answer the three questions raised above:

1. It is proved in Theorem 2.1 that a penalized procedure over the simplex satisfies the sharp oracle inequality (1.2) with  $\text{PRICE}_M(\delta) = c\sigma^2 \log(M/\delta)$  for some absolute constant  $c > 0$ . This price is of the same order as for the problem of aggregation of deterministic vectors. Thus the dependence between the estimators and the data used to aggregate them induces no extra cost.
2. The form of the affine estimators to aggregate has no impact on the price to pay for aggregation. In particular, the sharp oracle inequalities of the present paper do not involve quantities dependent on  $A_j$  such as  $\sigma^2 \text{Tr} A_j$ .

3. The only assumption made on the matrices  $A_1, \dots, A_M$  is that  $\|A_j\|_2 \leq 1$  for all  $j = 1, \dots, M$ , where  $\|\cdot\|_2$  is the operator norm. This assumption is natural and not restrictive since any admissible estimator of the form  $A\mathbf{y}$  has to satisfy  $\|A\|_2 \leq 1$  [1]. All other assumptions on the matrices  $A_1, \dots, A_M$  can be dropped, in particular the matrices can be non-symmetric and have negative eigenvalues.

The paper is organized as follows. In Section 1.1 we define the notation used throughout the paper. Section 2 defines a penalized procedure over the simplex and shows that it achieves sharp oracle inequalities in deviation for aggregation of affine estimators. The role of the penalty is studied in Section 3 and Section 4. Prior weights are considered in Section 5. Section 6 shows that the estimator is robust to variance misspecification and to non-Gaussianity of the noise. Some examples are given in Section 7. Section 8 is devoted to the proofs.

## 1.1 Notation

Let  $\mathbf{f} = (f_1, \dots, f_n)^T \in \mathbf{R}^n$  be an unknown regression vector. We observe  $n$  random variables (1.1) where  $\xi_1, \dots, \xi_n$  are subgaussian random variables, with  $\mathbb{E}[\xi_i] = 0$  and  $\mathbb{E}[\xi_i^2] = \sigma^2$ . It can be rewritten in the vector form  $\mathbf{y} = \mathbf{f} + \boldsymbol{\xi}$  where  $\mathbf{y} = (Y_1, \dots, Y_n)^T$ ,  $\mathbf{f} = (f_1, \dots, f_n)^T$  and  $\boldsymbol{\xi} = (\xi_1, \dots, \xi_n)^T$ .

For any estimator  $\hat{\boldsymbol{\mu}}$  of  $\mathbf{f}$ , we measure the quality of estimation of  $\mathbf{f}$  with the loss  $\|\hat{\boldsymbol{\mu}} - \mathbf{f}\|_2^2$ , where  $\|\cdot\|_2$  is the Euclidean norm in  $\mathbf{R}^n$ . Let  $M \geq 2$ . We consider  $M$  affine estimators of the form

$$\hat{\boldsymbol{\mu}}_j = A_j \mathbf{y} + \mathbf{b}_j, \quad j = 1, \dots, M.$$

The matrices  $A_1, \dots, A_M$  and the vectors  $\mathbf{b}_1, \dots, \mathbf{b}_M \in \mathbf{R}^n$  are deterministic. Define the simplex in  $\mathbf{R}^M$ :

$$\Lambda^M = \left\{ \boldsymbol{\theta} \in \mathbf{R}^M, \quad \sum_{j=1}^M \theta_j = 1, \quad \forall j = 1 \dots M, \quad \theta_j \geq 0 \right\}.$$

For any  $\boldsymbol{\theta} \in \Lambda^M$ , let

$$A_{\boldsymbol{\theta}} = \sum_{j=1}^M \theta_j A_j, \quad \mathbf{b}_{\boldsymbol{\theta}} = \sum_{j=1}^M \theta_j \mathbf{b}_j, \quad \hat{\boldsymbol{\mu}}_{\boldsymbol{\theta}} = A_{\boldsymbol{\theta}} \mathbf{y} + \mathbf{b}_{\boldsymbol{\theta}}.$$

Let  $\mathbf{e}_1, \dots, \mathbf{e}_M$  be the vectors of the canonical basis in  $\mathbf{R}^M$ . Then  $\hat{\boldsymbol{\mu}}_j = \hat{\boldsymbol{\mu}}_{\mathbf{e}_j}$  for all  $j = 1, \dots, M$ .

An orthoprojector is an  $n \times n$  matrix  $P$  such that

$$P = P^T = P^2. \quad (1.4)$$

Denote by  $I_{n \times n}$  the  $n \times n$ -identity matrix. For any  $n \times n$  real matrix  $A = (a_{i,j})_{i,j=1,\dots,n}$ , define the operator norm of  $A$ , the Frobenius (or Hilbert-Schmidt) norm of  $A$  and the nuclear norm of  $A$  respectively by:

$$\|A\|_2 = \sup_{x \neq 0} \frac{\|Ax\|_2}{\|x\|_2}, \quad \|A\|_F = \sqrt{\sum_{i,j=1,\dots,n} a_{i,j}^2}, \quad \|A\|_1 = \text{Tr}(\sqrt{A^T A}).$$

The following inequalities hold for any two squared matrices  $M, M'$ :

$$\|MM'\|_2 \leq \|M\|_2 \|M'\|_2, \quad \|MM'\|_F \leq \|M\|_2 \|M'\|_F. \quad (1.5)$$

Finally, denote by  $\log$  the natural logarithm with  $\log(e) = 1$ .

## 2 A penalized procedure on the simplex

For any  $\theta \in \Lambda^M$  define

$$C_p(\theta) := \|\hat{\mu}_\theta\|_2^2 - 2\mathbf{y}^T \hat{\mu}_\theta + 2\sigma^2 \text{Tr}(A_\theta), \quad (2.1)$$

which is the Mallows [32]  $C_p$ -criterion. Next, define

$$H_{\text{pen}}(\theta) = C_p(\theta) + \frac{1}{2} \text{pen}(\theta), \quad (2.2)$$

where

$$\text{pen}(\theta) = \sum_{j=1}^M \theta_j \|\hat{\mu}_\theta - \hat{\mu}_j\|_2^2. \quad (2.3)$$

We consider the estimator  $\hat{\mu}_{\hat{\theta}_{\text{pen}}}$  where

$$\hat{\theta}_{\text{pen}} \in \underset{\theta \in \Lambda^M}{\text{argmin}} H_{\text{pen}}(\theta). \quad (2.4)$$

The function  $H_{\text{pen}}$  is convex (cf. Lemma 8.1) and minimizing  $H_{\text{pen}}$  over the simplex is a quadratic program for which efficient algorithms are available. The convexity of  $H_{\text{pen}}$  also proves that  $\hat{\theta}_{\text{pen}}$  is well defined, although it may not be unique (for example if all  $\hat{\mu}_j$  are the same then  $H_{\text{pen}}$  is constant on the simplex).

We now explain the meaning of the terms that appear in (2.2). If  $\theta$  is fixed,  $C_p(\theta)$  is an unbiased estimate of the quantity

$$R(\theta) := \|\hat{\mu}_\theta\|_2^2 - 2\mathbf{f}^T \hat{\mu}_\theta = \|\hat{\mu}_\theta - \mathbf{f}\|_2^2 - \|\mathbf{f}\|_2^2, \quad (2.5)$$

which is the quantity of interest  $\|\hat{\mu}_\theta - \mathbf{f}\|_2^2$  up to the additive constant  $\|\mathbf{f}\|_2^2$ .

The penalty (2.3) is borrowed from the  $Q$ -aggregation procedure, which is a powerful tool to derive sharp oracle inequalities in deviation when the loss is strongly convex [36, 12, 30, 4]. Since the estimators  $\hat{\mu}_1, \dots, \hat{\mu}_M$  depend on the data, the penalty (2.3) is data-driven, which is not the case if  $\hat{\mu}_1, \dots, \hat{\mu}_M$  are deterministic vectors as in [12]. In order to give some geometric insights on the penalty (2.3), let  $c \in \mathbf{R}^n$  be a solution of  $M$  linear equations  $2c^T \hat{\mu}_j = \|\hat{\mu}_j\|_2^2, j = 1, \dots, M$ , and assume only in the rest of this paragraph that such a solution exists, even though this assumption cannot be fulfilled for  $M > n$ . Then

$$\text{pen}(\theta) = \sum_{j=1}^M \theta_j \|\hat{\mu}_j\|_2^2 - \|\hat{\mu}_\theta\|_2^2 = 2c^T \hat{\mu}_\theta - \|\hat{\mu}_\theta\|_2^2 = \|c\|_2^2 - \|\hat{\mu}_\theta - c\|_2^2. \quad (2.6)$$

Assume also only in this paragraph that the function  $\theta \rightarrow \hat{\mu}_\theta$  is bijective from the simplex  $\Lambda^M$  to the convex hull of  $\{\hat{\mu}_1, \dots, \hat{\mu}_M\}$ . Then we can write  $\text{pen}(\theta) = g(\hat{\mu}_\theta)$  for some function  $g$  defined on the convex hull of  $\{\hat{\mu}_1, \dots, \hat{\mu}_M\}$ . Equation (2.6) shows that the level sets of the function  $g$  are euclidean balls centered at  $c$ . The function  $g$  is non-negative, it is minimal at the extreme points  $\hat{\mu}_1, \dots, \hat{\mu}_M$  since  $g(\hat{\mu}_j) = 0$  for all  $j = 1, \dots, M$  and  $g$  is maximal at the projection of  $c$  on the convex hull of  $\{\hat{\mu}_1, \dots, \hat{\mu}_M\}$ . Intuitively, the penalty (2.3) pushes  $\theta$  away from the center of the simplex towards the vertices. Thus, the level sets of the function  $\theta \rightarrow \text{pen}(\theta)$  in  $\mathbf{R}^M$  are ellipsoids centered at  $\theta_c$ , where  $\theta_c$  is the unique point in  $\mathbf{R}^M$  such that  $\hat{\mu}_{\theta_c} = c$ . If  $M > n$  or if the vector  $c$  is not well defined, the level sets of  $\text{pen}(\cdot)$  are more intricate and cannot be described in such a simple way.

**Theorem 2.1** (Main result). *Let  $M \geq 2$ . For  $j = 1, \dots, M$ , consider the affine estimators  $\hat{\mu}_j = A_j \mathbf{y} + \mathbf{b}_j$  and assume that  $\|A_j\|_2 \leq 1$ . Assume that the noise random variables  $\xi_1, \dots, \xi_n$  are i.i.d.  $\mathcal{N}(0, \sigma^2)$ . Let  $\hat{\theta}_{\text{pen}}$  be the estimator defined in (2.4). Then for all  $x > 0$ , the estimator  $\hat{\mu}_{\hat{\theta}_{\text{pen}}}$  satisfies with probability greater than  $1 - 2 \exp(-x)$ ,*

$$\|\hat{\mu}_{\hat{\theta}_{\text{pen}}} - \mathbf{f}\|_2^2 \leq \min_{j=1, \dots, M} \|\hat{\mu}_j - \mathbf{f}\|_2^2 + 46\sigma^2(2 \log M + x). \quad (2.7)$$

Furthermore,

$$\mathbb{E} \|\hat{\mu}_{\hat{\theta}_{\text{pen}}} - \mathbf{f}\|_2^2 \leq \mathbb{E} \left[ \min_{j=1, \dots, M} \|\hat{\mu}_j - \mathbf{f}\|_2^2 \right] + 92\sigma^2 \log(eM). \quad (2.8)$$

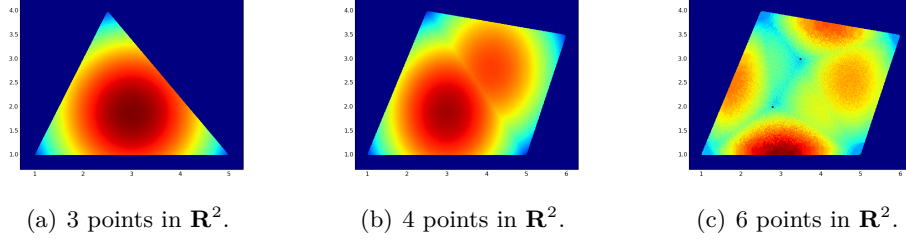


Figure 1: Penalty (2.3) heatmaps. Largest penalty in red, smallest in blue.

The sharp oracle inequality in deviation given in [13] presents an additive term proportional to  $\sigma^2 \text{Tr}(A_j)$ , as in (1.3). An improvement of the present paper is the absence of this additive term which can be large for matrices  $A_j$  with large trace. Our analysis shows that the quantities  $\sigma^2 \text{Tr}(A_j)$  are not meaningful for the problem of aggregation of affine estimators, and Theorem 2.1 improves upon the earlier result of [13].

We relax all assumptions on the matrices  $A_1, \dots, A_M$ , for instance they may be non-symmetric and have negative eigenvalues. Earlier works studied projection matrices [31], assumed some commutativity property of the matrices [14] or their symmetry and positive semi-definiteness [13]. Although it is shown in [11] that all admissible linear estimators correspond to symmetric  $A_j$  with non-negative eigenvalues, some linear estimators used in practice are not symmetric. For example, the last example of [14, Section 1.2] (“moving averages”), exhibits linear estimators that need not be symmetric: if two neighbors of the graph  $i, j$  have a different number of neighbours, then  $a_{ij} \neq a_{ji}$ . Our result also shows that the restrictions on the matrices  $A_1, \dots, A_M$  introduced in [31, 14, 13] are not intrinsic to the problem of aggregation of affine estimators.

For clarity we assume in Theorem 2.1 that the operator norm of each matrix is bounded by 1. This assumption is not restrictive since all admissible linear estimators of the form  $A\mathbf{y}$  satisfy  $\|A\|_2 \leq 1$  [11].

The next proposition shows that the bounds of Theorem 2.1 are optimal in a minimax sense. For any  $\mathbf{f} \in \mathbf{R}^n$  we denote by  $\mathbb{P}_{\mathbf{f}}$  the probability measure of the random variable  $\mathbf{y} = \mathbf{f} + \boldsymbol{\xi}$ . A lower bound for aggregation of deterministic vectors was proved in [37, Theorem 5.4 with  $S = 1$ ]. This lower bound implies the following result.

**Proposition 2.1.** *There exist absolute constants  $c^*, C^*, p^* > 0$  such that the following holds. For all  $M, n \geq C^*$ , there exist  $\mathbf{b}_1, \dots, \mathbf{b}_M \in \mathbf{R}^n$  and*



orthoprojectors  $A_1, \dots, A_M$  of rank one such that

$$\inf_{\hat{\boldsymbol{\mu}}} \sup_{\mathbf{f} \in \mathbf{R}^n} \mathbb{P}_{\mathbf{f}} \left( \|\hat{\boldsymbol{\mu}} - \mathbf{f}\|_2^2 - \min_{k=1, \dots, M} \|\mathbf{b}_k - \mathbf{f}\|_2^2 \geq c^* \sigma^2 \log(M) \right) \geq p^*, \quad (2.9)$$

$$\inf_{\hat{\boldsymbol{\mu}}} \sup_{\mathbf{f} \in \mathbf{R}^n} \mathbb{P}_{\mathbf{f}} \left( \|\hat{\boldsymbol{\mu}} - \mathbf{f}\|_2^2 - \min_{k=1, \dots, M} \|A_k \mathbf{y} - \mathbf{f}\|_2^2 \geq c^* \sigma^2 \log(M) \right) \geq p^*, \quad (2.10)$$

where the infima are taken over all estimators  $\hat{\boldsymbol{\mu}}$ .

This implies that the bounds of Theorem 2.1 are minimax optimal. The lower bound can be constructed either with a dictionary of deterministic vectors (cf. (2.9)), or with a dictionary of orthoprojectors of rank one (cf. (2.10)).

### 3 The penalty (2.3) improves upon model selection based on $C_p$

In order to explain the role of the penalty (2.3) for the problem of aggregation of affine estimators, consider first the standard empirical risk minimization scheme based on the  $C_p$  criterion. Define  $\hat{J}$  as

$$\hat{J} \in \operatorname{argmin}_{j=1, \dots, M} C_p(\mathbf{e}_j),$$

where  $C_p(\cdot)$  is defined in (2.1). Using that  $C_p(\mathbf{e}_{\hat{J}}) \leq C_p(\mathbf{e}_k)$  for all  $k = 1, \dots, M$  together with the definition of  $C_p(\cdot)$  and  $R(\cdot)$  given in (2.1) and (2.5), the following holds almost surely:

$$\|\hat{\boldsymbol{\mu}}_{\hat{J}} - \mathbf{f}\|_2^2 \leq \min_{k=1, \dots, M} \|\hat{\boldsymbol{\mu}}_k - \mathbf{f}\|_2^2 + \max_{j,k=1, \dots, M} \Delta_{jk}, \quad (3.1)$$

where  $\Delta_{jk} := C_p(\mathbf{e}_k) - C_p(\mathbf{e}_j) - (R(\mathbf{e}_k) - R(\mathbf{e}_j))$ . Thus, it is possible to prove an oracle inequality for the estimator  $\hat{\boldsymbol{\mu}}_{\hat{J}}$  if we can control the quantities  $\Delta_{jk}$  uniformly over all pairs  $j, k = 1, \dots, M$ . These quantities can be rewritten as

$$\Delta_{jk} = 2\boldsymbol{\xi}^T((A_j - A_k)\mathbf{f} + \mathbf{b}_j - \mathbf{b}_k) + 2\left(\boldsymbol{\xi}^T(A_j - A_k)\boldsymbol{\xi} - \sigma^2 \operatorname{Tr}(A_j - A_k)\right). \quad (3.2)$$

Two stochastic terms appear in  $\Delta_{jk}$ . The first is a centered Gaussian random variable with variance  $4\sigma^2\|(A_j - A_k)\mathbf{f} + \mathbf{b}_j - \mathbf{b}_k\|_2^2$ . The second is a centered quadratic form in  $\boldsymbol{\xi}$ , and it can be shown that its variance is of order  $\sigma^4\|A_j - A_k\|_{\mathbb{F}}^2$ . This quadratic term is sometimes called a Gaussian chaos of order 2. The deviations of these two terms are governed by the following

concentration inequalities. For any vector  $\mathbf{v} \in \mathbf{R}^n$ , a standard Gaussian tail bound gives

$$\mathbb{P}(\mathbf{v}^T \boldsymbol{\xi} > \sigma \|\mathbf{v}\|_2 \sqrt{2x}) \leq \exp(-x), \quad \forall x > 0. \quad (3.3)$$

For the Gaussian chaos of order 2, the following is proved in [9, Example 2.12].

**Lemma 3.1.** *Assume that  $\boldsymbol{\xi} \sim \mathcal{N}(0, \sigma^2 I_{n \times n})$ . For any squared matrix  $B$  of size  $n$ ,*

$$\mathbb{P}(\boldsymbol{\xi}^T B \boldsymbol{\xi} - \sigma^2 \text{Tr} B > 2\sigma^2 \|B\|_F \sqrt{x} + 2\sigma^2 \|B\|_2 x) \leq \exp(-x), \quad (3.4)$$

where  $\sigma^2 \text{Tr} B = \mathbb{E}[\boldsymbol{\xi}^T B \boldsymbol{\xi}]$ .

We set  $\mathbf{v} = 2((A_j - A_k)\mathbf{f} + \mathbf{b}_j - \mathbf{b}_k)$  and  $B = 2(A_k - A_j)$  to study the deviations of the random variable  $\Delta_{jk}$ . If  $\|A_j - A_k\|_2$  is small, (3.3) and (3.4) yield that the deviations of  $\Delta_{jk}$  are of order of the two quantities

$$\sigma \|(A_j - A_k)\mathbf{f} + \mathbf{b}_j - \mathbf{b}_k\|_2, \quad \sigma^2 \|A_j - A_k\|_F, \quad (3.5)$$

i.e., the standard deviations of the two terms in  $\Delta_{jk}$ . The concentration inequalities (3.3) and (3.4) are known to be tight [28], thus there is little hope to bound the deviations of  $\Delta_{jk}$  independently of  $\mathbf{f}$ ,  $A_j$  and  $A_k$  in order to prove a sharp oracle inequality. It is possible to refine the above analysis and to prove the following oracle inequality, though with a leading constant greater than 1.

**Proposition 3.1.** *There exist absolute constants  $c, C > 0$  such that the following holds. Assume that  $\|A_j\|_2 \leq 1$  for all  $j = 1, \dots, M$ . Let  $0 < \epsilon < c$ . For all  $x > 0$ , the estimator  $\hat{\boldsymbol{\mu}}_j$  defined above satisfies with probability greater than  $1 - 2\exp(-x)$*

$$\|\hat{\boldsymbol{\mu}}_j - \mathbf{f}\|_2^2 \leq (1 + \epsilon) \min_{k=1, \dots, M} \|\hat{\boldsymbol{\mu}}_k - \mathbf{f}\|_2^2 + C\sigma^2(x + 2\log M)/\epsilon.$$

The proof of Proposition 3.1 is given in the supplementary material. The estimator  $\hat{\boldsymbol{\mu}}_j$  fails to achieve a sharp oracle inequality with a remainder term of order  $\sigma^2 \log M$ , and this drawback cannot be repaired for all procedures of the form  $\hat{\boldsymbol{\mu}}_{\hat{K}}$  where  $\hat{K}$  is an estimator valued in  $\{1, \dots, M\}$ . Indeed, it is proved in [20, Section 6.4.2 and Proposition 6.1] that there exist  $\mathbf{f}_1, \mathbf{f}_2 \in \mathbf{R}^n$  and orthoprojectors  $A_1, A_2$  such that for any estimator  $\hat{K}$  valued in  $\{1, 2\}$ ,

$$\sup_{\mathbf{f} \in \{\mathbf{f}_1, \mathbf{f}_2\}} \left( \mathbb{E} \|A_{\hat{K}} \mathbf{y} - \mathbf{f}\|_2^2 - \min_{j=1,2} \mathbb{E} \|A_j \mathbf{y} - \mathbf{f}\|_2^2 \right) \geq \sigma^2 \sqrt{n}/4, \quad (3.6)$$

provided that  $n$  is larger than some absolute constant. Inspection of the proof of this result reveals that

$$\sigma\|(A_2 - A_1)\mathbf{f} + \mathbf{b}_2 - \mathbf{b}_1\|_2 \geq \sigma^2\sqrt{n}, \quad \forall \mathbf{f} \in \{\mathbf{f}_1, \mathbf{f}_2\},$$

where we set  $\mathbf{b}_1 = \mathbf{b}_2 = 0$ . Thus, this lower bound of order  $\sqrt{n}$  is related to the Gaussian component of the random variable  $\Delta_{12}$ , i.e., to the term  $\boldsymbol{\xi}^T((A_1 - A_2)\mathbf{f} + \mathbf{b}_1 - \mathbf{b}_2)$ , cf. (3.2).

The procedure  $\hat{\boldsymbol{\mu}}_j$  fails to achieve a sharp oracle inequality because the variances of the two components of  $\Delta_{jk}$  may be large and cannot be controlled. The role of the penalty (2.3) is exactly to control the deviations of  $\Delta_{jk}$  by controlling the terms (3.5). The following proposition makes this precise.

**Proposition 3.2.** *Let  $\hat{\boldsymbol{\theta}}_{\text{pen}}$  be the estimator (2.4). Then almost surely,*

$$\|\hat{\boldsymbol{\mu}}_{\hat{\boldsymbol{\theta}}_{\text{pen}}} - \mathbf{f}\|_2^2 \leq \min_{q=1,\dots,M} (\|\hat{\boldsymbol{\mu}}_q - \mathbf{f}\|_2^2) + \max_{j,k=1,\dots,M} \left( \Delta_{jk} - \frac{1}{2} \|\hat{\boldsymbol{\mu}}_j - \hat{\boldsymbol{\mu}}_k\|_2^2 \right), \quad (3.7)$$

where  $\Delta_{jk}$  is the quantity (3.2). Furthermore, for all  $j, k = 1, \dots, M$ ,

$$\mathbb{E} \left[ \frac{1}{2} \|\hat{\boldsymbol{\mu}}_j - \hat{\boldsymbol{\mu}}_k\|_2^2 \right] = \frac{1}{2} \|(A_j - A_k)\mathbf{f} + \mathbf{b}_j - \mathbf{b}_k\|_2^2 + \frac{\sigma^2}{2} \|A_j - A_k\|_{\text{F}}^2. \quad (3.8)$$

The proof of Proposition 3.2 is a simple consequence of the KKT conditions for the minimization problem (2.4). Compared with (3.1), the right hand side of (3.7) presents the quantities  $\frac{1}{2} \|\hat{\boldsymbol{\mu}}_j - \hat{\boldsymbol{\mu}}_k\|_2^2$ . We will explain below that these quantities appear because of the interplay between the penalty (2.3) and the strong convexity of  $H_{\text{pen}}$ .

The second part of Proposition 3.2 states that for each  $j, k$ , the quantity  $\mathbb{E} \frac{1}{2} \|\hat{\boldsymbol{\mu}}_j - \hat{\boldsymbol{\mu}}_k\|_2^2$  is the sum of two terms, which are exactly the variances of the two stochastic terms in  $\Delta_{jk}$ , cf. (3.2). This explains the success of the penalty (2.3) for the problem of model selection type aggregation: the penalty and the strong convexity of  $H_{\text{pen}}$  provide the quantity  $\frac{1}{2} \|\hat{\boldsymbol{\mu}}_j - \hat{\boldsymbol{\mu}}_k\|_2^2$ , and this quantity is exactly what is needed to control the deviations of the random variable  $\Delta_{jk}$ .

## 4 Strong convexity and the penalty (2.3)

To further understand the interplay between the penalty (2.3) and the strong convexity of  $H_{\text{pen}}$ , we now give an outline of the proof of (3.7). Let

$k = 1, \dots, M$  be fixed. For any  $\boldsymbol{\theta} \in \Lambda^M$ , it will be useful to define the quantity

$$\Delta_k(\boldsymbol{\theta}) = 2\boldsymbol{\xi}^T((A_{\boldsymbol{\theta}} - A_k)\mathbf{f} + \mathbf{b}_j - \mathbf{b}_k) + 2\left(\boldsymbol{\xi}^T(A_{\boldsymbol{\theta}} - A_k)\boldsymbol{\xi} - \sigma^2\text{Tr}(A_{\boldsymbol{\theta}} - A_k)\right). \quad (4.1)$$

The function  $\Delta_k(\cdot)$  is affine in  $\boldsymbol{\theta}$  and for all  $j = 1, \dots, M$ , we have  $\Delta_k(\mathbf{e}_j) = \Delta_{jk}$ . The KKT conditions for the optimization problem (2.4) and  $\text{pen}(\mathbf{e}_k) = 0$  imply that

$$\|\hat{\boldsymbol{\mu}}_{\hat{\boldsymbol{\theta}}_{\text{pen}}} - \mathbf{f}\|_2^2 \leq \|\hat{\boldsymbol{\mu}}_k - \mathbf{f}\|_2^2 + \Delta_k(\hat{\boldsymbol{\theta}}_{\text{pen}}) - \frac{1}{2} \left[ \text{pen}(\hat{\boldsymbol{\theta}}_{\text{pen}}) + \|\hat{\boldsymbol{\mu}}_{\hat{\boldsymbol{\theta}}_{\text{pen}}} - \hat{\boldsymbol{\mu}}_k\|_2^2 \right].$$

The term  $\|\hat{\boldsymbol{\mu}}_{\hat{\boldsymbol{\theta}}_{\text{pen}}} - \hat{\boldsymbol{\mu}}_k\|_2^2$  comes from the strong convexity of the function  $H_{\text{pen}}$ . Thanks to (8.1) with  $\mathbf{g} = \hat{\boldsymbol{\mu}}_k$ , we have the bias-variance decomposition

$$\text{pen}(\hat{\boldsymbol{\theta}}_{\text{pen}}) + \underbrace{\|\hat{\boldsymbol{\mu}}_{\hat{\boldsymbol{\theta}}_{\text{pen}}} - \hat{\boldsymbol{\mu}}_k\|_2^2}_{\text{Term given by the strong convexity of } H_{\text{pen}}} = \sum_{j=1}^M \hat{\theta}_{\text{pen},j} \underbrace{\|\hat{\boldsymbol{\mu}}_j - \hat{\boldsymbol{\mu}}_k\|_2^2}_{\text{Term that controls the deviations of } \Delta_{jk}}. \quad (4.2)$$

Now, the function  $\boldsymbol{\theta} \rightarrow \Delta_k(\boldsymbol{\theta}) - \sum_{j=1}^M \theta_j \|\hat{\boldsymbol{\mu}}_j - \hat{\boldsymbol{\mu}}_k\|_2^2$  is affine in  $\boldsymbol{\theta}$ , thus it is maximized at a vertex of the simplex and

$$\Delta_k(\hat{\boldsymbol{\theta}}_{\text{pen}}) - \frac{1}{2} \left[ \text{pen}(\hat{\boldsymbol{\theta}}_{\text{pen}}) + \|\hat{\boldsymbol{\mu}}_{\hat{\boldsymbol{\theta}}_{\text{pen}}} - \hat{\boldsymbol{\mu}}_k\|_2^2 \right] \leq \max_{j,k=1,\dots,M} \left( \Delta_{jk} - \frac{1}{2} \|\hat{\boldsymbol{\mu}}_k - \hat{\boldsymbol{\mu}}_j\|_2^2 \right).$$

The sketch of the proof of (3.7) is complete.

The strong convexity of  $C_p(\cdot)$  and  $H_{\text{pen}}(\cdot)$  will be understood with respect to the pseudometric

$$\|\hat{\boldsymbol{\mu}}_{\boldsymbol{\theta}} - \hat{\boldsymbol{\mu}}_{\boldsymbol{\theta}'}\|_2, \quad \boldsymbol{\theta}, \boldsymbol{\theta}' \in \mathbf{R}^M,$$

so it is not the strong convexity in the Euclidean norm. We say that a function  $V(\cdot)$  is strongly convex with coefficient  $\gamma > 0$  over the simplex if for all  $\boldsymbol{\theta}, \boldsymbol{\theta}' \in \Lambda^M$ ,

$$V(\boldsymbol{\theta}) \geq V(\boldsymbol{\theta}') + \nabla V(\boldsymbol{\theta}')^T(\boldsymbol{\theta} - \boldsymbol{\theta}') + \gamma \|\hat{\boldsymbol{\mu}}_{\boldsymbol{\theta}} - \hat{\boldsymbol{\mu}}_{\boldsymbol{\theta}'}\|_2^2.$$

The strong convexity of  $H_{\text{pen}}$  could be used because  $H_{\text{pen}}$  is minimized over the simplex and not just over the vertices. Indeed, minimizing a strongly convex function over a discrete set, as in the definition of  $\hat{J}$ , only grants the inequalities

$$C_p(\mathbf{e}_j) \leq C_p(\mathbf{e}_k), \quad \text{for all } k = 1, \dots, M.$$

Because the simplex is a convex set, minimizing the strongly convex function  $H_{\text{pen}}$  over the simplex grants the inequalities

$$H_{\text{pen}}(\hat{\boldsymbol{\theta}}_{\text{pen}}) \leq H_{\text{pen}}(\boldsymbol{\theta}) - \frac{1}{2} \|\hat{\boldsymbol{\mu}}_{\boldsymbol{\theta}} - \hat{\boldsymbol{\mu}}_{\hat{\boldsymbol{\theta}}_{\text{pen}}}\|_2^2, \quad \text{for all } \boldsymbol{\theta} \in \Lambda^M.$$

One could also consider the estimator  $\hat{\boldsymbol{\theta}}_C \in \operatorname{argmin}_{\boldsymbol{\theta} \in \Lambda^M} C_p(\boldsymbol{\theta})$ . Because of the strong convexity of  $C_p(\cdot)$ , this estimator enjoys the inequalities

$$C_p(\hat{\boldsymbol{\theta}}_C) \leq C_p(\boldsymbol{\theta}) - \|\hat{\boldsymbol{\mu}}_{\boldsymbol{\theta}} - \hat{\boldsymbol{\mu}}_{\hat{\boldsymbol{\theta}}_{\text{pen}}}\|_2^2, \quad \text{for all } \boldsymbol{\theta} \in \Lambda^M.$$

The above displays highlight the fact that  $C_p(\cdot)$  and  $H_{\text{pen}}(\cdot)$  have different strong convexity coefficients. This is because  $H_{\text{pen}}(\cdot) = C_p(\cdot) + (1/2) \text{pen}(\cdot)$  and  $(1/2) \text{pen}(\cdot)$  is strongly concave with coefficient  $1/2$ , thus the strong convexity coefficient of  $H_{\text{pen}}(\cdot)$  is less than the one of  $C_p(\cdot)$ . We refer to Lemma 8.1 for a rigorous proof of the strong convexity of  $H_{\text{pen}}$  and  $C_p$ . Formula (4.2) highlights another feature of the penalty (2.3): the penalty transforms the quadratic term given by strong convexity into the linear term given by the right hand side of (4.2).

The estimator  $\hat{\boldsymbol{\mu}}_{\hat{\boldsymbol{\theta}}_C}$  is another candidate for the problem of aggregation of affine estimators. It is close to the estimator  $\hat{\boldsymbol{\mu}}_{\hat{\boldsymbol{\theta}}_{\text{pen}}}$ , except that the penalty (2.3) has been removed from the function to minimize. It was proved in [12, Section 2.2] that when  $A_j = 0$  for all  $j = 1, \dots, M$ , this estimator performs poorly: for large enough  $M$  and  $n$ , there exist  $\mathbf{f}$  and  $\mathbf{b}_1, \dots, \mathbf{b}_M \in \mathbf{R}^n$  such that with probability greater than  $1/4$ ,

$$\|\hat{\boldsymbol{\mu}}_{\hat{\boldsymbol{\theta}}_C} - \mathbf{f}\|_2^2 \geq \min_{j=1, \dots, M} \|\hat{\boldsymbol{\mu}}_j - \mathbf{f}\|_2^2 + \frac{\sigma^2 \sqrt{n}}{48},$$

where  $\hat{\boldsymbol{\mu}}_j = \mathbf{b}_j$  for all  $j = 1, \dots, M$ .

## 5 Prior weights

We consider now the problem of aggregation of  $M$  affine estimators with a prior probability distribution  $\boldsymbol{\pi} = (\pi_1, \dots, \pi_M)^T$  on the finite set of indices  $\{1, \dots, M\}$ .

**Theorem 5.1.** *Let  $M \geq 2$ . For  $j = 1, \dots, M$ , consider the estimator  $\hat{\boldsymbol{\mu}}_j = A_j \mathbf{y} + \mathbf{b}_j$  and assume that  $\|A_j\|_2 \leq 1$ . Let  $\boldsymbol{\pi} = (\pi_1, \dots, \pi_M)^T \in \Lambda^M$ . Assume that the noise  $\boldsymbol{\xi}$  has distribution  $\mathcal{N}(0, \sigma^2 I_{n \times n})$ . Let  $\hat{\boldsymbol{\theta}}_{\boldsymbol{\pi}} \in \operatorname{argmin}_{\boldsymbol{\theta} \in \Lambda^M} V_{\text{pen}}(\boldsymbol{\theta})$  where*

$$V_{\text{pen}}(\boldsymbol{\theta}) := H_{\text{pen}}(\boldsymbol{\theta}) + 46\sigma^2 \sum_{j=1}^M \theta_j \log \frac{1}{\pi_j}. \quad (5.1)$$

Then for all  $x > 0$ , with probability greater than  $1 - 2\exp(-x)$ ,

$$\|\hat{\boldsymbol{\mu}}_{\hat{\boldsymbol{\theta}}_\pi} - \mathbf{f}\|_2^2 \leq \min_{j=1,\dots,M} \left( \|\hat{\boldsymbol{\mu}}_j - \mathbf{f}\|_2^2 + 92\sigma^2 \log \frac{1}{\pi_j} \right) + 46\sigma^2 x. \quad (5.2)$$

The prior probability distribution  $\boldsymbol{\pi} = (\pi_j)_{j=1,\dots,M}$  is deterministic and does not depend on the data  $\mathbf{y} = (Y_1, \dots, Y_n)^T$ . The only difference between the function (2.2) and the function minimized in (5.1) is the term

$$\sigma^2 \sum_{j=1}^M \theta_j \log \frac{1}{\pi_j}. \quad (5.3)$$

This term allows us to weight the candidates  $\hat{\boldsymbol{\mu}}_1, \dots, \hat{\boldsymbol{\mu}}_M$  with the prior probability distribution  $(\pi_j)_{j=1,\dots,M}$  based on some prior knowledge about the estimators  $\hat{\boldsymbol{\mu}}_1, \dots, \hat{\boldsymbol{\mu}}_M$ . For example, if the estimators are orthoprojectors, one can set prior weights that decrease with the rank the orthoprojectors [37, 38]. The same term is used in [30] whereas [13] uses the Kullback-Leibler divergence of  $\boldsymbol{\theta}$  from  $\boldsymbol{\pi}$ . It is shown in [12] that for aggregation of deterministic vectors, one may use a quantity of the form  $\sum_{j=1}^M \theta_j \log(\rho(\theta_j)/\pi_j)$  where  $\rho(\cdot)$  satisfies  $\rho(t) \geq t$  and  $t \rightarrow t \log(\rho(t))$  is convex. This suggests that we could use the Kullback-Leibler divergence of  $\boldsymbol{\theta}$  from  $\boldsymbol{\pi}$  instead of (5.3), but in their current form our proofs only hold with the “linear entropy” (5.3).

## 6 Robustness of the estimator $\hat{\boldsymbol{\mu}}_{\hat{\boldsymbol{\theta}}_{\text{pen}}}$

We prove in this section that the procedure (2.4) is robust to non Gaussian noise distributions and to variance misspecification.

### 6.1 Robustness to non-Gaussian noise

The following result shows that the penalized procedure (2.4) is robust to non-Gaussian noise distributions.

**Theorem 6.1.** *Let  $M \geq 2$ . Let  $\bar{\sigma} > 0$ . For  $j = 1, \dots, M$ , consider the estimator  $\hat{\boldsymbol{\mu}}_j = A_j \mathbf{y} + \mathbf{b}_j$  and assume that  $\|A_j\|_2 \leq 1$ . Assume that the noise components  $\xi_1, \dots, \xi_n$  are i.i.d., centered with variance  $\sigma^2$  and satisfy for all  $\mathbf{b} \in \mathbf{R}^n$ , all matrices  $B$  and all  $x > 0$*

$$\mathbb{P}(\boldsymbol{\xi}^T \mathbf{b} > \bar{\sigma} \sqrt{2x}) \leq \exp(-x), \quad (6.1)$$

$$\mathbb{P}(\boldsymbol{\xi}^T B \boldsymbol{\xi} - \sigma^2 \text{Tr} B > 2\sigma \bar{\sigma} \|B\|_F \sqrt{x} + 2\bar{\sigma}^2 \|B\|_2 x) \leq \exp(-x). \quad (6.2)$$

Let  $\hat{\boldsymbol{\theta}}_{\text{pen}}$  be the estimator defined in (2.4). Then for all  $x > 0$ , the estimator  $\hat{\boldsymbol{\mu}}_{\hat{\boldsymbol{\theta}}_{\text{pen}}}$  satisfies with probability greater than  $1 - 2\exp(-x)$ ,

$$\|\hat{\boldsymbol{\mu}}_{\hat{\boldsymbol{\theta}}_{\text{pen}}} - \mathbf{f}\|_2^2 \leq \min_{j=1,\dots,M} \|\hat{\boldsymbol{\mu}}_j - \mathbf{f}\|_2^2 + 46\bar{\sigma}^2(2\log M + x). \quad (6.3)$$

Let  $K > 0$ . If the random variables  $\xi_1, \dots, \xi_n$  are i.i.d., centered with variance  $\sigma^2$  and  $K$ -subgaussian in the sense that  $\log \mathbb{E}[e^{t\xi_i}] \leq K^2 t^2/2$  for all  $t \in \mathbf{R}$  and all  $i = 1, \dots, n$ , then (6.1) is satisfied with  $\bar{\sigma} = cK$  for some absolute constant  $c > 0$  [44, Section 5.2.3]. As  $\sigma \leq K$ , (6.1) is also satisfied with  $\bar{\sigma} = cK^2/\sigma$ . By the Hanson-Wright inequality [24, 45, 39], (6.2) also holds with  $\bar{\sigma} = cK^2/\sigma$  for another absolute constant  $c > 0$ . Thus, for i.i.d.  $K$ -subgaussian random variables with variance  $\sigma^2$ , (6.3) yields

$$\|\hat{\boldsymbol{\mu}}_{\hat{\boldsymbol{\theta}}_{\text{pen}}} - \mathbf{f}\|_2^2 \leq \min_{j=1,\dots,M} \|\hat{\boldsymbol{\mu}}_j - \mathbf{f}\|_2^2 + C(K^4/\sigma^2)(2\log M + x), \quad (6.4)$$

for some absolute constant  $C > 0$ . For most common examples of subgaussian random variables, the standard deviation  $\sigma$  is of the same order as the subgaussian norm  $K$ , so the bound (6.4) is satisfying. This bound may not be tight if the standard deviation is pathologically small compared to the subgaussian norm.

## 6.2 Robustness to variance misspecification

In order to construct the estimator (2.4) by minimizing (2.2), the knowledge of the variance of the noise is needed. However, the following proposition shows that the procedure (2.4) is robust to variance misspecification, i.e., the result still holds if the variance is replaced by an estimator  $\hat{\sigma}^2$  as soon as  $\hat{\sigma}^2$  is consistent in a weak sense defined below.

**Theorem 6.2** (Aggregation under variance misspecification). *Let  $M \geq 2$ . For  $j = 1, \dots, M$ , consider the estimator  $\hat{\boldsymbol{\mu}}_j = A_j \mathbf{y} + \mathbf{b}_j$ . Assume that the noise random variables  $\xi_1, \dots, \xi_n$  are i.i.d.  $\mathcal{N}(0, \sigma^2)$ . Let  $\hat{\sigma}^2$  be an estimator and assume that*

$$\forall j = 1, \dots, M, A_j = A_j^T = A_j^2, \quad \delta := \mathbb{P}(|\sigma^2 - \hat{\sigma}^2| > \sigma^2/8) < 1. \quad (6.5)$$

Let  $\hat{\boldsymbol{\theta}}_{\hat{\sigma}} = \operatorname{argmin}_{\boldsymbol{\theta} \in \Lambda^M} W_{\text{pen}}(\boldsymbol{\theta})$  where

$$W_{\text{pen}}(\boldsymbol{\theta}) := \|\hat{\boldsymbol{\mu}}_{\boldsymbol{\theta}}\|_2^2 - 2\mathbf{y}^T \hat{\boldsymbol{\mu}}_{\boldsymbol{\theta}} + 2\hat{\sigma}^2 \operatorname{Tr}(A_{\boldsymbol{\theta}}) + \frac{1}{2} \operatorname{pen}(\boldsymbol{\theta}). \quad (6.6)$$

Then for all  $x > 0$ , with probability greater than  $1 - \delta - 2\exp(-x)$ ,

$$\|\hat{\boldsymbol{\mu}}_{\hat{\boldsymbol{\theta}}_{\hat{\sigma}}} - \mathbf{f}\|_2^2 \leq \min_{j=1,\dots,M} \|\hat{\boldsymbol{\mu}}_j - \mathbf{f}\|_2^2 + 64\sigma^2(x + 2\log M).$$

The proof of Theorem 6.2 is given in Section 8.2. In (6.5), the matrices  $A_1, \dots, A_M$  are assumed to be orthoprojectors, so Theorem 6.2 is a result for aggregation of Least Squares estimators. As soon as an estimator  $\hat{\sigma}^2$  satisfies with high probability  $|\hat{\sigma}^2 - \sigma^2| \leq \sigma^2/8$ , optimal aggregation of Least Squares estimators is possible. This condition is weaker than consistency, as any estimator  $\hat{\sigma}^2$  that converges to  $\sigma^2$  in probability satisfies this condition for  $n$  large enough.

The proof of Theorem 6.2 exploits the form of the penalty (2.3) and the strong convexity of the function (6.6). Similarly to Proposition 3.2, we will prove that almost surely,

$$\begin{aligned} \|\hat{\boldsymbol{\mu}}_{\hat{\sigma}^2} - \mathbf{f}\|_2^2 &\leq \min_{q=1, \dots, M} \|\hat{\boldsymbol{\mu}}_q - \mathbf{f}\|_2^2 \\ &+ \max_{j, k=1, \dots, M} \left( \Delta_{jk} - \frac{1}{2} \|\hat{\boldsymbol{\mu}}_j - \hat{\boldsymbol{\mu}}_k\|_2^2 + 2(\sigma^2 - \hat{\sigma}^2) \text{Tr}(A_j - A_k) \right), \end{aligned} \quad (6.7)$$

where  $\Delta_{jk}$  is the quantity (3.2). The only difference from (3.7) is in the extra term  $2(\sigma^2 - \hat{\sigma}^2) \text{Tr}(A_j - A_k)$  that appears because we used  $\hat{\sigma}^2$  instead of  $\sigma^2$  in the definition of  $W_{\text{pen}}(\cdot)$ . On the event  $|\hat{\sigma}^2 - \sigma^2| \leq \sigma^2/8$ , it is easy to check that (cf. Lemma 8.2)

$$2(\sigma^2 - \hat{\sigma}^2) \text{Tr}(A_j - A_k) \leq \frac{\sigma^2}{4} \|A_j - A_k\|_{\text{F}}^2.$$

As explained in the discussion that follows Proposition 3.2, the quantity  $\frac{1}{2} \|\hat{\boldsymbol{\mu}}_j - \hat{\boldsymbol{\mu}}_k\|_2^2$  is given by the interplay between the penalty (2.3) and the strong convexity of the function that is minimized. By (3.8), the expectation of this quantity is greater than  $(\sigma^2/2) \|A_j - A_k\|_{\text{F}}^2$ . Thus, the penalty (2.3) and the strong convexity of  $W_{\text{pen}}$  provide exactly what is needed to compensate the difference between  $\hat{\sigma}^2$  and  $\sigma^2$ . Hence, the proof of Theorem 6.2 reveals that the robustness to variance misspecification is in fact due to the interplay between the penalty (2.3) and the strong convexity of  $W_{\text{pen}}$ .

The papers [21, 22, 3] aim at performing aggregation of Least Squares estimators when  $\sigma^2$  is unknown, but unlike Theorem 6.2 the oracle inequalities that they established have a leading constant greater than 1. To our knowledge, Theorem 6.2 is the first aggregation result, with leading constant 1, that is robust to variance misspecification.

In the following, we describe several situations where the suitable estimator  $\hat{\sigma}^2$  is available.

*Example 6.1* (An estimator  $\hat{\sigma}^2$  that does not depend on  $\mathbf{y}$ ). In [14, Section 3.1], two contexts are given where an unbiased estimator of the covariance



matrix, independent from  $\mathbf{y}$ , is available. For example, the noise level can be estimated independently if the signal is captured multiple times by a single device, or if several identical devices capture the same signal.

*Example 6.2* (Difference based estimators). In nonparametric regression where the non-random design points are equispaced in  $[0, 1]$ , a well known estimator of the noise level is the difference based estimator  $1/(2n-2) \sum_{i=1}^{n-1} (y_{i+1} - y_i)^2$ . This technique can be refined with more complex difference sequences [23, 16], and extends to design points in a multidimensional space [33]. For images, where the underlying space is 2-dimensional, there exist efficient methods which require no multiplication [26].

*Example 6.3* (Consistent estimation of  $\sigma^2$  in high-dimensional linear regression). In a high-dimensional setting, it is possible to estimate  $\sigma^2$  under classical assumptions in high-dimensional regression. First, the scaled LASSO [40] allows a joint estimation of the regression coefficients and of the noise level  $\sigma^2$ . The estimator  $\hat{\sigma}^2$  of the scaled LASSO converges in probability to the true noise level  $\sigma^2$  [40, Theorem 1], and  $\hat{\sigma}^2/\sigma^2$  is asymptotically normal [40, Equation (19)]. Second, [5] proposes to estimate  $\sigma^2$  with a recursive procedure that uses LASSO residuals, and non-asymptotic guarantees are proved [5, Supplementary material]. Third, [6] provides non-asymptotic bounds on the estimation of  $\sigma^2$  by the residuals of the Square-Root LASSO [6, Theorem 2] and these bounds imply consistency. In Theorem 6.2, we require that  $|\hat{\sigma}^2/\sigma^2 - 1| \leq 1/8$  with high-probability and this requirement is far weaker than the guarantees obtained in [5, 40].

## 7 Examples

### 7.1 Adaptation to the smoothness

For all  $n \geq 1$ , given continuous parameters  $\beta \geq 1$  and  $L > 0$ , we consider subsets  $\Theta(\beta, L) \subset \mathbf{R}^n$ . We assume that for each  $\beta \geq 1$ , there exists a squared matrix  $A_\beta$  of size  $n$  with  $\|A_\beta\|_2 \leq 1$  such that for all  $L > 0$ , as  $n \rightarrow +\infty$ ,

$$\inf_{\hat{\mathbf{f}}} \sup_{\mathbf{f} \in \Theta(\beta, L)} \frac{1}{n} \mathbb{E} \|\mathbf{f} - \hat{\mathbf{f}}\|_2^2 \sim \sup_{\mathbf{f} \in \Theta(\beta, L)} \frac{1}{n} \mathbb{E} \|\mathbf{f} - A_\beta \mathbf{y}\|_2^2 \sim C^* n^{\frac{-2\beta}{2\beta+1}}, \quad (7.1)$$

where  $a_n \sim b_n$  if and only if  $a_n/b_n \rightarrow 1$  as  $n \rightarrow +\infty$ , the infimum is taken over all estimators and the constant  $C^* > 0$  may depend on  $\beta, L$  and  $\sigma$ . The above assumption holds for Sobolev ellipsoids in nonparametric regression, and in this case one can choose the Pinsker filters for the matrices  $A_\beta$  (cf.

[43, Theorem 3.2]). For Sobolev ellipsoids, there exist different estimators that adapt to the unknown smoothness. [19, 43, 14]

Consider the following aggregation procedure. Assume that  $n \geq 3$  and let  $M = \lceil 120 \log(n)(\log \log n)^2 \rceil$ . For all  $j = 1, \dots, M$ , let  $\beta_j = (1 + 1/(\log(n) \log \log n))^{j-1}$ . We aggregate the linear estimators  $(\hat{\boldsymbol{\mu}}_j = A_{\beta_j} \mathbf{y})_{j=1, \dots, M}$  using the procedure (2.4) of Theorem 2.1, and denote by  $\tilde{\boldsymbol{\mu}}$  the resulting estimator. The following adaptation result is a direct consequence of Theorem 2.1.

**Proposition 7.1.** *For all  $n \geq 3$ ,  $\beta \geq 1$  and  $L > 0$ , let  $\Theta(\beta, L) \subset \mathbf{R}^n$  such that as  $n \rightarrow +\infty$ , (7.1) is satisfied for some matrices  $A_\beta$  with  $\|A_\beta\|_2 \leq 1$ . Assume that the sets  $\Theta(\beta, L)$  are ordered, i.e.,  $\Theta(\beta, L) \subset \Theta(\beta', L)$  for any  $\beta > \beta'$  and any  $L > 0$ . For all  $\beta \geq 1$  and  $L > 0$ , the estimator  $\tilde{\boldsymbol{\mu}}$  defined above satisfies as  $n \rightarrow +\infty$*

$$\lim_{n \rightarrow +\infty} \sup_{\mathbf{f} \in \Theta(\beta, L)} \frac{1}{n} \mathbb{E} \|\mathbf{f} - \tilde{\boldsymbol{\mu}}\|_2^2 n^{\frac{2\beta}{2\beta+1}} = C^*.$$

The above procedure adapts to the unknown smoothness in exact asymptotic sense by aggregating only  $\log(n)(\log \log n)^2$  estimators so its computational complexity is small. Another feature is that the minimax rate and the minimax constant  $C^*$  are not altered by the aggregation step.

## 7.2 The best convex combination as a benchmark

We consider convex combinations of the estimators  $\hat{\boldsymbol{\mu}}_1, \dots, \hat{\boldsymbol{\mu}}_M$  to construct the estimator (2.4). The goal of this section is to study the performance of the estimator (2.4) if the benchmark is  $\min_{\boldsymbol{\theta} \in \Lambda^M} \|\hat{\boldsymbol{\mu}}_{\boldsymbol{\theta}} - \mathbf{f}\|_2^2$  instead of  $\min_{k=1, \dots, M} \|\hat{\boldsymbol{\mu}}_k - \mathbf{f}\|_2^2$ .

The penalty (2.3) vanishes at the extreme points:  $\text{pen}(\mathbf{e}_j) = 0$  for all  $j = 1, \dots, M$ , and it pushes  $\hat{\boldsymbol{\mu}}_{\hat{\boldsymbol{\theta}}_{\text{pen}}}$  towards the points  $\{\hat{\boldsymbol{\mu}}_1, \dots, \hat{\boldsymbol{\mu}}_M\}$ . This can be seen in Figure 1. Consider a noise-free problem where  $\sigma = 0$ . Let  $\mathbf{f} \in \mathbf{R}^n$ . Consider estimators  $\hat{\boldsymbol{\mu}}_1, \dots, \hat{\boldsymbol{\mu}}_M$  such that  $\|\hat{\boldsymbol{\mu}}_j\|_2^2 = \rho > 0$  for all  $j = 1, \dots, M$  (here, the estimators are deterministic because  $\sigma = 0$ ). Then  $\text{pen}(\boldsymbol{\theta}) = \rho - \|\hat{\boldsymbol{\mu}}_{\boldsymbol{\theta}}\|_2^2$  and  $H_{\text{pen}}(\boldsymbol{\theta}) = (1/2)\|\hat{\boldsymbol{\mu}}_{\boldsymbol{\theta}} - 2\mathbf{f}\|_2^2 + c$  where  $c$  is constant that depends on  $\rho$  and  $\mathbf{f}$  but not on  $\boldsymbol{\theta}$ . If both  $\mathbf{f}$  and  $2\mathbf{f}$  lie in the convex hull of  $\hat{\boldsymbol{\mu}}_1, \dots, \hat{\boldsymbol{\mu}}_M$ ,  $\hat{\boldsymbol{\mu}}_{\hat{\boldsymbol{\theta}}}$  defined in (2.4) will be equal to  $2\mathbf{f}$  instead of  $\mathbf{f}$  and is likely to be a bad procedure with respect to the benchmark  $\min_{\boldsymbol{\theta} \in \Lambda^M} \|\hat{\boldsymbol{\mu}}_{\boldsymbol{\theta}} - \mathbf{f}\|_2^2$ . This fact is not surprising since the penalty penalizes heavily some regions of the convex hull of the estimators. Furthermore this procedure is tailored for the benchmark  $\min_{k=1, \dots, M} \|\hat{\boldsymbol{\mu}}_k - \mathbf{f}\|_2^2$  and its goal is not to mimic the best convex combination of the estimators.

It is possible to modify the procedure (2.4) to construct an estimator that performs well with respect to the best convex combination of  $M$  linear estimators. Let

$$m := \left\lfloor \sqrt{\frac{n}{\log(1 + M/\sqrt{n})}} \right\rfloor. \quad (7.2)$$

If  $m \geq 1$ , define the set  $\Lambda_m^M \subset \Lambda^M$  as

$$\Lambda_m^M := \left\{ \frac{1}{m} \sum_{q=1}^m \mathbf{u}_q, \quad \mathbf{u}_1, \dots, \mathbf{u}_m \in \{\mathbf{e}_1, \dots, \mathbf{e}_M\} \right\}. \quad (7.3)$$

Denote by  $|\Lambda_m^M|$  the cardinality of  $\Lambda_m^M$ . We aggregate the affine estimators  $(\hat{\boldsymbol{\mu}}_{\mathbf{u}})_{\mathbf{u} \in \Lambda_m^M}$  using the procedure (2.4) and denote by  $\hat{\boldsymbol{\mu}}_{\Lambda_m^M}$  the resulting estimator.

**Proposition 7.2.** *Let  $M, n \geq 1$ . For  $j = 1, \dots, M$ , consider the estimator  $\hat{\boldsymbol{\mu}}_j = A_j \mathbf{y} + \mathbf{b}_j$  for any  $n \times n$  matrix  $A_j$  and vector  $\mathbf{b}_j \in \mathbf{R}^n$ . Assume that  $\boldsymbol{\xi} \sim N(0, \sigma^2 I_{n \times n})$  and that for some constant  $R > 0$ ,*

$$\frac{1}{n} \|\mathbf{f}\|_2^2 \leq R^2, \quad \frac{1}{n} \|\mathbf{b}_j\|_2^2 \leq R^2, \quad \|A_j\|_2 \leq 1, \quad \forall j = 1, \dots, M.$$

*For all  $x > 0$ , the estimator  $\hat{\boldsymbol{\theta}}_C \in \operatorname{argmin}_{\boldsymbol{\theta} \in \Lambda^M} C_p(\boldsymbol{\theta})$  satisfies with probability greater than  $1 - 2 \exp(-x)$ ,*

$$\frac{1}{n} \|\hat{\boldsymbol{\mu}}_{\hat{\boldsymbol{\theta}}_C} - \mathbf{f}\|_2^2 \leq \min_{\boldsymbol{\theta} \in \Lambda^M} \frac{1}{n} \|\hat{\boldsymbol{\mu}}_{\boldsymbol{\theta}} - \mathbf{f}\|_2^2 + 8(\sigma^2 + \sigma R \sqrt{2}) \sqrt{\frac{x + 2 \log M}{n}} + \frac{8\sigma^2(x + 2 \log M)}{n}. \quad (7.4)$$

*If  $M \leq \sqrt{n}(\exp(n) - 1)$  then for all  $x > 0$ , the estimator  $\hat{\boldsymbol{\mu}}_{\Lambda_m^M}$  defined above satisfies with probability greater than  $1 - 3 \exp(-x)$ ,*

$$\frac{1}{n} \|\hat{\boldsymbol{\mu}}_{\Lambda_m^M} - \mathbf{f}\|_2^2 \leq \min_{\boldsymbol{\theta} \in \Lambda^M} \frac{1}{n} \|\hat{\boldsymbol{\mu}}_{\boldsymbol{\theta}} - \mathbf{f}\|_2^2 + C \max(R^2, \sigma^2) \sqrt{\frac{\log(1 + M/\sqrt{n})}{n}} + \frac{C\sigma^2 x}{n}. \quad (7.5)$$

To our knowledge, this is the first result that provides a sharp oracle inequality for the problem of aggregation of affine estimators with respect to the convex oracle. However, there is a large literature on convex aggregation when the estimators to aggregate are deterministic, which corresponds to the particular case  $A_j = 0$  for all  $j = 1, \dots, M$ . When the error is measured with the scaled squared norm  $\frac{1}{n} \|\cdot\|_2^2$ , the minimax rate of convex aggregation is known to be of order  $M/n$  if  $M \leq \sqrt{n}$  and  $\sqrt{\log(1 + M/\sqrt{n})/n}$  if  $M > \sqrt{n}$ .

For our setting, this is proved in [37]. This elbow effect was first established for regression with random design [42] and then extended to other settings in [35, 36]. All these results assume that the estimators to aggregate are deterministic or independent of the data used for aggregation. The lower bound [37, Theorem 5.3 with  $S = M$ ,  $\delta = \sigma$  and  $R = \log(1 + eM)$ ] yields that there exist absolute constants  $c, C > 0$  such that if  $\log(1 + eM)^2 \leq Cn$ , there exist deterministic vectors  $\hat{\boldsymbol{\mu}}_1 = \mathbf{b}_1, \dots, \hat{\boldsymbol{\mu}}_M = \mathbf{b}_M$  such that for all estimators  $\hat{\boldsymbol{\mu}}$ ,

$$\sup_{\mathbf{f} \in \mathbf{R}^n} \mathbb{P}_{\mathbf{f}} \left( \frac{1}{n} \|\hat{\boldsymbol{\mu}} - \mathbf{f}\|_2^2 - \min_{\boldsymbol{\theta} \in \Lambda^M} \frac{1}{n} \|\hat{\boldsymbol{\mu}}_{\boldsymbol{\theta}} - \mathbf{f}\|_2^2 \geq c\sigma^2 \left( \frac{M}{n} \wedge \sqrt{\frac{\log(1 + M/\sqrt{n})}{n}} \right) \right) \geq c.$$

Thus, if  $M \geq \sqrt{n}$ , (7.5) is optimal in a minimax sense up to absolute constants, and (7.4) is optimal up to logarithmic factors. However, we do not know whether the minimax rate is  $M/n$  when  $M < \sqrt{n}$ , as in the case of aggregation of deterministic vectors.

The problem of linear aggregation of affine estimators remains open. It is only known that for linear aggregation of deterministic vectors, the Least Squares estimator on a linear space of dimension  $M$  achieves the rate  $\sigma^2 M/n$ , which is optimal in a minimax sense [42, 35, 37, 36].

### 7.3 $k$ -regressors

Let  $\mathbb{X}$  be a design matrix consisting of  $p$  columns and  $n$  rows. Let  $k$  be an integer such that  $1 \leq k \leq n$ . Consider the family of distinct estimators  $\{\hat{\boldsymbol{\mu}}_1, \dots, \hat{\boldsymbol{\mu}}_M\}$  where for each  $j = 1, \dots, M$ ,  $\hat{\boldsymbol{\mu}}_j = A_j \mathbf{y}$  and  $A_j$  is the orthoprojector on a linear span of  $k$  linearly independent columns of  $\mathbb{X}$ . In particular,  $M \leq \binom{p}{k}$ . The estimator  $\hat{\boldsymbol{\mu}}_j$  is the Least Squares estimator on the subspace  $V_j$  of dimension  $k$  which is the linear span of these  $k$  columns.

Now consider the estimator  $\hat{\boldsymbol{\theta}}^{(k)} \in \mathbf{R}^M$  defined by

$$\hat{\boldsymbol{\theta}}^{(k)} = \operatorname{argmin}_{\boldsymbol{\theta} \in \Lambda^M} \left( \|\hat{\boldsymbol{\mu}}_{\boldsymbol{\theta}} - \mathbf{y}\|_2^2 + \frac{1}{2} \operatorname{pen}(\boldsymbol{\theta}) \right),$$

where  $\operatorname{pen}(\cdot)$  is the penalty (2.3). It is exactly the procedure (2.4) from Theorem 2.1 since the projection matrices  $A_1, \dots, A_M$  have the same trace equal to  $k$ . This procedure is fully adaptive with respect to the unknown variance of the noise. The following result is a direct consequence of Theorem 2.1. The estimator  $\hat{\boldsymbol{\theta}}^{(k)}$  satisfies for all  $x > 0$ , with probability greater

than  $1 - 3 \exp(-x)$ ,

$$\|\hat{\boldsymbol{\mu}}_{\boldsymbol{\theta}^{(k)}} - \mathbf{f}\|_2^2 \leq \min_{\boldsymbol{\beta} \in \mathbf{R}^p, |\boldsymbol{\beta}|_0 \leq k} \|\mathbb{X}\boldsymbol{\beta} - \mathbf{f}\|_2^2 + c\sigma^2 \left( k \log \left( \frac{ep}{k} \right) + x \right),$$

for some absolute constant  $c > 0$ .

## 7.4 Sparsity pattern aggregation

Given a design matrix  $\mathbb{X}$  with  $p$  columns, an estimator  $\hat{\boldsymbol{\mu}}$  of  $\mathbf{f}$  is said to achieve a sparsity oracle inequality if it satisfies

$$\|\hat{\boldsymbol{\mu}} - \mathbf{f}\|_2^2 \leq \min_{\boldsymbol{\theta} \in \mathbf{R}^p} \left( C \|\mathbb{X}\boldsymbol{\theta} - \mathbf{f}\|_2^2 + \Delta(|\boldsymbol{\theta}|_0) \right), \quad (7.6)$$

with high probability or in expectation. In (7.6),  $C \geq 1$ ,  $|\boldsymbol{\theta}|_0$  is the number of non-zero coefficients of  $\boldsymbol{\theta}$  and  $\Delta$  is an increasing function, which may also depend on problem parameters such as the variance of the noise or the design matrix  $\mathbb{X}$ . See (7.7) below for a typical example of such function  $\Delta(\cdot)$ . Results of the form (7.6) are of major interest in high-dimensional statistics where the number of covariates  $p$  exceeds the number of observations [37]. First approach to get such results can be found in [18], and in an expanded form in [7, 8], under Gaussian noise with a leading constant  $C > 1$ . The drawback of having  $C > 1$  cannot be repaired for these penalized model selection procedures (cf. (3.6) and [20, Section 6.4.2]). More recently, aggregation methods based on exponential weights [37, 38, 41] and then  $Q$ -aggregation [13] were shown to achieve sharp oracle inequalities similar to (7.6). These sharp oracle inequalities were proved for Gaussian noise with known variance.

Aggregation procedures with prior weights [15, 12, 30, 4] as in Theorem 5.1 can be used to prove sparsity oracle inequalities if sparsity-inducing prior weights are used. For instance, sparsity pattern aggregation [37, 38, 13, 41] leads to the following oracle inequality. Given a design matrix  $\mathbb{X}$  with  $p$  columns, there exists an estimator  $\hat{\boldsymbol{\mu}}$  that satisfies with probability greater than  $1 - 2 \exp(-x)$ ,

$$\|\hat{\boldsymbol{\mu}} - \mathbf{f}\|_2^2 \leq \min_{\boldsymbol{\theta} \in \mathbf{R}^p} \left( \|\mathbb{X}\boldsymbol{\theta} - \mathbf{f}\|_2^2 + c\sigma^2 |\boldsymbol{\theta}|_0 \log \left( \frac{ep}{1 \vee |\boldsymbol{\theta}|_0} \right) \right) + c'\sigma^2 x, \quad (7.7)$$

where  $c, c' > 0$  are absolute constants and  $|\boldsymbol{\theta}|_0$  denotes the number of non-zero coefficients of  $\boldsymbol{\theta}$ . When the noise is Gaussian, the result (7.7) is proved in [13] and a similar result in expectation was shown in [37, 41].

We now derive a similar result for subgaussian noise. We propose below a new sparsity pattern aggregation method that only requires an estimator  $\hat{K}^2$

that upper bounds the subgaussian norm of the noise with high probability. We will make the following assumption on the noise. For some constant  $K > 0$ , we assume that the random vector  $\boldsymbol{\xi}$  satisfies:

$$\forall \alpha \in \mathbf{R}^n, \quad \mathbb{E} \exp(\alpha^T \boldsymbol{\xi}) \leq \exp\left(\frac{\|\alpha\|_2^2 K^2}{2}\right). \quad (7.8)$$

As opposed to the previous section, the components of  $\boldsymbol{\xi}$  are not assumed to be independent.

For each subset  $J \subset \{1, \dots, p\}$ , let  $\hat{\boldsymbol{\mu}}_J^{LS}$  be the Least Squares estimator on the linear span of the columns of  $\mathbb{X}$  whose indices are in  $J$ . The estimator  $\hat{\boldsymbol{\mu}}_J^{LS}$  is of the form  $\hat{\boldsymbol{\mu}}_J^{LS} = A_J \mathbf{y}$  for some projection matrix  $A_J$ . Consider the weights  $\pi_J \propto e^{-|J|} \binom{p}{|J|}^{-1}$  and choose the normalisation constant such that  $\sum_{J \subseteq \{1, \dots, p\}} \pi_J = 1$ . Given  $\boldsymbol{\lambda} = (\lambda_J)_{J \subseteq \{1, \dots, p\}}$ , let  $\hat{\boldsymbol{\mu}}_{\boldsymbol{\lambda}} = \sum_{J \subseteq \{1, \dots, p\}} A_J \mathbf{y}$ . Let  $\hat{\boldsymbol{\mu}}_{\text{SPA}} = \hat{\boldsymbol{\mu}}_{\hat{\boldsymbol{\lambda}}}$  where  $\hat{\boldsymbol{\lambda}} = (\hat{\lambda}_J)_{J \subseteq \{1, \dots, p\}}$  is a minimizer of

$$\|\mathbf{y} - \hat{\boldsymbol{\mu}}_{\boldsymbol{\lambda}}\|_2^2 + \sum_{J \subseteq \{1, \dots, p\}} \lambda_J \left( \frac{1}{2} \|A_J \mathbf{y} - \hat{\boldsymbol{\mu}}_{\boldsymbol{\lambda}}\|_2^2 + 32 \hat{K}^2 \log \frac{1}{\pi_J} \right)$$

over the set

$$\Lambda = \left\{ \boldsymbol{\lambda} = (\lambda_J)_{J \subseteq \{1, \dots, p\}}, \quad \sum_{J \subseteq \{1, \dots, p\}} \lambda_J = 1, \quad \lambda_J \geq 0, \forall J \subseteq \{1, \dots, p\} \right\}.$$

As sparsity pattern aggregation is not central in the present paper, we keep this presentation short and refer the reader to [37, 38, 13, 41] for more details on sparsity pattern aggregation and the construction of Least Squares estimators.

Then the following sparsity oracle inequality holds, where  $|\boldsymbol{\theta}|_0$  is the number of non-zero coefficients of  $\boldsymbol{\theta}$ .

**Theorem 7.1.** *Let  $\mathbb{X}$  be a deterministic design matrix with  $p$  columns. Let  $K > 0$  be the smallest positive real number such that the noise random  $\boldsymbol{\xi}$  satisfies (7.8). Let  $\hat{K}$  be a given estimator and let  $\delta := \mathbb{P}(\hat{K}^2 < K^2)$ . Then, the estimator  $\hat{\boldsymbol{\mu}}_{\text{SPA}}$  defined above satisfies with probability greater than  $1 - \delta - 3 \exp(-x)$ ,*

$$\begin{aligned} \|\hat{\boldsymbol{\mu}}_{\text{SPA}} - \mathbf{f}\|_2^2 &\leq \inf_{\boldsymbol{\theta} \in \mathbf{R}^p} \left[ \|\mathbb{X}\boldsymbol{\theta} - \mathbf{f}\|_2^2 + 31K^2x \right. \\ &\quad \left. + (64\hat{K}^2 + 4K^2) \left( \frac{1}{2} + 2|\boldsymbol{\theta}|_0 \log \left( \frac{ep}{1 \vee |\boldsymbol{\theta}|_0} \right) \right) \right]. \quad (7.9) \end{aligned}$$

Theorem 7.1 is proved in the supplementary material. It improves upon the previous results on sparsity pattern aggregation [13, 37, 38, 41] in several aspects.

First, the noise  $\xi$  is only assumed to be subgaussian and its components need not be independent, whereas previous results only hold under Gaussianity and independence of the noise components [13, 37, 38, 41]. Theorem 7.1 shows that the optimal bounds are of the same form in this more general setting.

Second, to construct the aggregates in [13, 37, 38, 41] one needs the exact knowledge of the covariance matrix of the noise. In Theorem 7.1, only an upper bound of the subgaussian norm of the noise is needed to construct the estimator.

Third, we do not split the data in order to perform sparsity pattern aggregation, as opposed to the “sample cloning” approach [41, Lemma 2.1]. Sample cloning is possible only for Gaussian noise when the variance is known; it cannot be used here as  $\xi$  can be any subgaussian vector.

The estimator of Theorem 7.1 achieves the minimax rate for any intersection of  $\ell_0$  and  $\ell_q$  balls, where  $q \in (0, 2)$ . This can be shown by applying the arguments of [13, 41] and bounding the right hand side of (7.9). Indeed, although [13, 41] consider only normal random variables, the argument does not depend on the noise distribution.

The result above holds without any assumption on the design matrix  $\mathbb{X}$ , as opposed to the LASSO or the Dantzig estimators which need assumptions on the design matrix  $\mathbb{X}$  to achieve sparsity oracle inequalities similar but weaker than (7.9).

The interest of the LASSO and the Dantzig estimators is that they can be computed efficiently for large  $p$ . The sparsity pattern aggregate based on exponential weights can also be computed efficiently using MCMC methods [37]. The estimator  $\hat{\theta}^{SPA}$  proposed here suffers the same drawback as [7] or the sparsity pattern aggregate performed with  $Q$ -aggregation [13]: it is not known whether these estimators can be computed in polynomial time, which makes them useful only for relatively small  $p$ .

## 8 Proofs

### 8.1 Proof of the main results

The penalty (2.3) satisfies for any  $\mathbf{g} \in \mathbf{R}^n$  and any  $\boldsymbol{\theta} \in \Lambda^M$ :

$$\sum_{k=1}^M \theta_k \|\hat{\boldsymbol{\mu}}_k - \mathbf{g}\|_2^2 = \|\hat{\boldsymbol{\mu}}_{\boldsymbol{\theta}} - \mathbf{g}\|_2^2 + \text{pen}(\boldsymbol{\theta}). \quad (8.1)$$

This can be shown by using simple properties of the Euclidean norm, or by noting that the equality above is a bias-variance decomposition. For  $\mathbf{g} = 0$ , (8.1) yields  $\text{pen}(\boldsymbol{\theta}) = -\|\hat{\boldsymbol{\mu}}_{\boldsymbol{\theta}}\|_2^2 + \sum_{k=1}^M \theta_k \|\hat{\boldsymbol{\mu}}_k\|_2^2$ .

**Lemma 8.1.** *Let  $F$  be any one of the functions  $H_{\text{pen}}$ ,  $V_{\text{pen}}$ ,  $W_{\text{pen}}$  or  $U$  defined in (2.2), (5.1), (6.6) and the supplementary material, respectively. Then  $F$  is convex, differentiable and satisfies for all  $\boldsymbol{\theta}, \boldsymbol{\theta}_0 \in \Lambda^M$ ,*

$$F(\boldsymbol{\theta}) = F(\boldsymbol{\theta}_0) + \nabla F(\boldsymbol{\theta}_0)^T (\boldsymbol{\theta} - \boldsymbol{\theta}_0) + \frac{1}{2} \|\hat{\boldsymbol{\mu}}_{\boldsymbol{\theta}} - \hat{\boldsymbol{\mu}}_{\boldsymbol{\theta}_0}\|_2^2. \quad (8.2)$$

Furthermore, if  $\hat{\boldsymbol{\theta}}$  is a minimizer of  $F$  over the simplex then for all  $\boldsymbol{\theta} \in \Lambda^M$ ,

$$F(\boldsymbol{\theta}) \geq F(\hat{\boldsymbol{\theta}}) + \frac{1}{2} \|\hat{\boldsymbol{\mu}}_{\boldsymbol{\theta}} - \hat{\boldsymbol{\mu}}_{\hat{\boldsymbol{\theta}}}\|_2^2. \quad (8.3)$$

*Proof.* Using (8.1) with  $\mathbf{g} = 0$  we obtain that the function  $F$  is a polynomial of degree 2, of the form  $F(\boldsymbol{\theta}) = \text{affine}(\boldsymbol{\theta}) + \frac{1}{2} \|\hat{\boldsymbol{\mu}}_{\boldsymbol{\theta}}\|_2^2$  where  $\text{affine}(\cdot)$  is an affine function of  $\boldsymbol{\theta}$ . This shows that  $F$  is convex and differentiable. The result (8.2) follows by uniqueness of the Taylor expansion of  $F$  (or by an explicit calculation of  $\nabla F(\boldsymbol{\theta}_0)$ ). Inequality (8.3) is a consequence of [10, 4.2.3, equation (4.21)].  $\square$

*Proof of Proposition 3.2.* Let  $\hat{\boldsymbol{\theta}} = \hat{\boldsymbol{\theta}}_{\text{pen}}$  for notational simplicity. Let  $q = 1, \dots, M$ . Inequality (8.3) with  $F = H_{\text{pen}}$  and  $\boldsymbol{\theta} = \mathbf{e}_q$  can be rewritten

$$0 \leq \|\hat{\boldsymbol{\mu}}_q - \mathbf{f}\|_2^2 - \|\hat{\boldsymbol{\mu}}_{\hat{\boldsymbol{\theta}}} - \mathbf{f}\|_2^2 - 2\boldsymbol{\xi}^T (\hat{\boldsymbol{\mu}}_q - \hat{\boldsymbol{\mu}}_{\hat{\boldsymbol{\theta}}}) + 2\sigma^2 \text{Tr}(A_q - A_{\hat{\boldsymbol{\theta}}}) \\ \frac{1}{2} [\text{pen}(\hat{\boldsymbol{\theta}}) + \|\hat{\boldsymbol{\mu}}_{\hat{\boldsymbol{\theta}}} - \hat{\boldsymbol{\mu}}_q\|_2^2].$$

Using (4.2) which is a consequence of (8.1) with  $\mathbf{g} = \hat{\boldsymbol{\mu}}_q$ , the previous display becomes

$$\|\hat{\boldsymbol{\mu}}_{\hat{\boldsymbol{\theta}}} - \mathbf{f}\|_2^2 \leq \|\hat{\boldsymbol{\mu}}_q - \mathbf{f}\|_2^2 + \Delta_q(\hat{\boldsymbol{\theta}}) - \frac{1}{2} \sum_{k=1}^M \hat{\theta}_k \|\hat{\boldsymbol{\mu}}_q - \hat{\boldsymbol{\mu}}_k\|_2^2,$$



where  $\Delta_q(\cdot)$  is defined in (4.1). For all  $q = 1, \dots, M$  and  $\boldsymbol{\theta} \in \Lambda^M$ , let  $Z(q, \boldsymbol{\theta}) := \Delta_q(\boldsymbol{\theta}) - \frac{1}{2} \sum_{k=1}^M \theta_k \|\hat{\boldsymbol{\mu}}_q - \hat{\boldsymbol{\mu}}_k\|_2^2$ . The quantity  $Z(q, \boldsymbol{\theta})$  is affine in its second argument  $\boldsymbol{\theta} \in \Lambda^M$  thus it is maximized at a vertex of  $\Lambda^M$ , and the following upper bounds hold:

$$Z(q, \hat{\boldsymbol{\theta}}) \leq \max_{\boldsymbol{\theta} \in \Lambda^M} Z(q, \boldsymbol{\theta}) = \max_{k=1, \dots, M} Z(q, \mathbf{e}_k) \leq \max_{j, k=1, \dots, M} Z(j, \mathbf{e}_k).$$

This completes the proof of (3.7). A bias-variance decomposition directly yields (3.8), since  $\mathbb{E}[\hat{\boldsymbol{\mu}}_j - \hat{\boldsymbol{\mu}}_k] = (A_j - A_k)\mathbf{f} + \mathbf{b}_j - \mathbf{b}_k$  and

$$\mathbb{E}\|\hat{\boldsymbol{\mu}}_j - \hat{\boldsymbol{\mu}}_k - \mathbb{E}[\hat{\boldsymbol{\mu}}_j - \hat{\boldsymbol{\mu}}_k]\|_2^2 = \mathbb{E}\|(A_j - A_k)\boldsymbol{\xi}\|_2^2 = \sigma^2 \|A_j - A_k\|_F^2.$$

□

The following notation will be useful. Define for all  $j, k = 1, \dots, M$

$$Q_{j,k} := \left(2I_{n \times n} - \frac{1}{2}(A_k - A_j)^T\right)(A_k - A_j), \quad (8.4)$$

$$\mathbf{v}_{j,k} := \left(2I_{n \times n} - (A_k - A_j)^T\right)((A_k - A_j)\mathbf{f} + \mathbf{b}_k - \mathbf{b}_j). \quad (8.5)$$

Let  $B_{jk} = A_k - A_j$ , so that  $\hat{\boldsymbol{\mu}}_k - \hat{\boldsymbol{\mu}}_j = B_{jk}\boldsymbol{\xi} + (B_{jk}\mathbf{f} + \mathbf{b}_k - \mathbf{b}_j)$ . Then

$$\|\hat{\boldsymbol{\mu}}_k - \hat{\boldsymbol{\mu}}_j\|_2^2 = \|B_{jk}\boldsymbol{\xi}\|_2^2 + \|B_{jk}\mathbf{f} + \mathbf{b}_k - \mathbf{b}_j\|_2^2 + 2\boldsymbol{\xi}^T B_{jk}^T (B_{jk}\mathbf{f} + \mathbf{b}_k - \mathbf{b}_j).$$

Thus, simple algebra yields that

$$\begin{aligned} \Delta_{jk} - \frac{1}{2}\|\hat{\boldsymbol{\mu}}_k - \hat{\boldsymbol{\mu}}_j\|_2^2 &= \boldsymbol{\xi}^T Q_{j,k} \boldsymbol{\xi} - \mathbb{E}[\boldsymbol{\xi}^T Q_{j,k} \boldsymbol{\xi}] + \boldsymbol{\xi}^T \mathbf{v}_{j,k} \\ &\quad - \frac{\sigma^2}{2} \|B_{jk}\|_F^2 - \frac{1}{2} \|B_{jk}\mathbf{f} + \mathbf{b}_k - \mathbf{b}_j\|_2^2 \end{aligned} \quad (8.6)$$

where we used the equality  $\sigma^2 \|B_{jk}\|_F^2 = \mathbb{E}[\|B_{jk}\boldsymbol{\xi}\|_2^2]$  and the above definitions of  $Q_{j,k}$  and  $\mathbf{v}_{j,k}$ .

*Proof of Theorem 2.1.* For all  $j, k = 1, \dots, M$ , using (1.5) and  $\|A_j\|_2 \leq 1$  we have

$$\begin{aligned} \|Q_{j,k}\|_2 &\leq 6, \quad \|Q_{j,k}\|_F \leq 3 \|A_k - A_j\|_F, \\ \|\mathbf{v}_{j,k}\|_2 &\leq 4 \|(A_k - A_j)\mathbf{f} + \mathbf{b}_k - \mathbf{b}_j\|_2. \end{aligned} \quad (8.7)$$

We apply (3.4) to the matrix  $Q_{j,k}$  and (3.3) to the vector  $\mathbf{v}_{j,k}$ . For all  $x > 0$ , it yields that on an event  $\Omega_{j,k}(x)$  of probability greater than  $1 - 2\exp(-x)$ ,

$$\begin{aligned}\boldsymbol{\xi}^T Q_{j,k} \boldsymbol{\xi} - \mathbb{E}[\boldsymbol{\xi}^T Q_{j,k} \boldsymbol{\xi}] &\leq \sigma^2(12x + 6\|A_k - A_j\|_F \sqrt{x}), \\ &\leq 30\sigma^2 x + \frac{\sigma^2}{2} \|A_k - A_j\|_F^2, \\ \text{and } \boldsymbol{\xi}^T \mathbf{v}_{j,k} &\leq \sigma 4\|(A_k - A_j)\mathbf{f} + \mathbf{b}_k - \mathbf{b}_j\|_2 \sqrt{2x}, \\ &\leq 16\sigma^2 x + \frac{1}{2} \|(A_k - A_j)\mathbf{f} + \mathbf{b}_k - \mathbf{b}_j\|_2^2, \quad (8.8)\end{aligned}$$

where we used twice the simple inequality  $2st \leq s^2 + t^2$ . In summary, we have proved that for any fixed pair  $(j, k)$ ,  $\Delta_{jk} - \frac{1}{2}\|\hat{\boldsymbol{\mu}}_j - \hat{\boldsymbol{\mu}}_k\|_2^2 \leq 46\sigma^2 x$  with probability greater than  $1 - 2\exp(-x)$ . By the union bound, this holds uniformly over all pairs  $j, k = 1, \dots, M$  with probability greater than  $1 - 2M^2 \exp(-x)$ . Set  $x' = x - 2\log(M)$ . Combining this bound with (6.7) and (8.6) completes the proof of (2.7).

We obtain (2.8) by integration as follows. Let  $Z$  be the positive part of the random variable  $(\|\hat{\boldsymbol{\mu}}_{\hat{\boldsymbol{\theta}}_{\text{pen}}} - \mathbf{f}\|_2^2 - \min_{j=1, \dots, M} \|\hat{\boldsymbol{\mu}}_j - \mathbf{f}\|_2^2) / (46\sigma^2) - 2\log M$ . We have  $\mathbb{P}(Z > x) \leq 2\exp(-x)$ , thus  $\mathbb{E}Z = \int_0^\infty \mathbb{P}(Z > x) dx \leq 2$ .  $\square$

*Proof of Theorem 6.1.* We proceed similarly to the proof of Theorem 2.1 above. For a fixed pair  $(j, k)$ , we apply (6.1) to the vector  $\mathbf{v}_{j,k}$  and (6.2) to the matrix  $Q_{j,k}$ . Using (8.7),

$$\begin{aligned}\boldsymbol{\xi}^T Q_{j,k} \boldsymbol{\xi} - \mathbb{E}[\boldsymbol{\xi}^T Q_{j,k} \boldsymbol{\xi}] &\leq \bar{\sigma}^2 12x + 6\sigma\bar{\sigma} \|A_k - A_j\|_F \sqrt{x}, \\ &\leq 30\bar{\sigma}^2 x + \frac{\sigma^2}{2} \|A_k - A_j\|_F^2, \\ \boldsymbol{\xi}^T \mathbf{v}_{j,k} &\leq \bar{\sigma} 4\|(A_k - A_j)\mathbf{f} + \mathbf{b}_k - \mathbf{b}_j\|_2 \sqrt{2x}, \\ &\leq 16\bar{\sigma}^2 x + \frac{1}{2} \|(A_k - A_j)\mathbf{f} + \mathbf{b}_k - \mathbf{b}_j\|_2^2.\end{aligned}$$

Combining this bound with (6.7), (8.6) and the union bound completes the proof.  $\square$

*Proof of Theorem 5.1.* Let  $\beta = 46\sigma^2$ . Let  $\hat{\boldsymbol{\theta}} = \hat{\boldsymbol{\theta}}_\pi$  for notational simplicity. The only difference between  $H_{\text{pen}}$  and  $V_{\text{pen}}$  is the linear term (5.3). Let  $q = 1, \dots, M$ . Inequality (8.3) with  $F = V_{\text{pen}}$  and  $\boldsymbol{\theta} = \mathbf{e}_q$  can be rewritten

$$\begin{aligned}\|\hat{\boldsymbol{\mu}}_{\hat{\boldsymbol{\theta}}_\pi} - \mathbf{f}\|_2^2 &\leq \|\hat{\boldsymbol{\mu}}_q - \mathbf{f}\|_2^2 + 2\beta \log(1/\pi_q) \\ &\quad + \Delta_q(\hat{\boldsymbol{\theta}}) - \frac{1}{2} \sum_{k=1}^M \hat{\theta}_k \|\hat{\boldsymbol{\mu}}_q - \hat{\boldsymbol{\mu}}_k\|_2^2 - \beta \sum_{k=1}^M \hat{\theta}_k \log \frac{1}{\pi_q \pi_k}. \quad (8.9)\end{aligned}$$

The second line is affine in  $\hat{\boldsymbol{\theta}}$  and is maximized at a vertex. It is upper bounded by

$$\max_{j,k=1,\dots,M} \left( \Delta_{jk} - \frac{1}{2} \|\hat{\boldsymbol{\mu}}_j - \hat{\boldsymbol{\mu}}_k\|_2^2 - \beta \log \frac{1}{\pi_j \pi_k} \right). \quad (8.10)$$

Fix a pair  $(j, k)$ . We proved in the proof of Theorem 2.1 above that with probability greater than  $1 - 2 \exp(-x)$ ,

$$\Delta_{jk} - \frac{1}{2} \|\hat{\boldsymbol{\mu}}_j - \hat{\boldsymbol{\mu}}_k\|_2^2 \leq \beta x.$$

Let  $x' = x - \log(1/(\pi_j \pi_k))$ . Then with probability greater than  $1 - 2\pi_j \pi_k \exp(-x')$ ,

$$\Delta_{jk} - \frac{1}{2} \|\hat{\boldsymbol{\mu}}_j - \hat{\boldsymbol{\mu}}_k\|_2^2 - \beta \log \frac{1}{\pi_j \pi_k} \leq \beta x'. \quad (8.11)$$

For all  $x' > 0$ , the bound (8.11) holds uniformly over all pairs  $j, k = 1, \dots, M$  with probability greater than

$$1 - 2 \sum_{j,k=1,\dots,M} \pi_j \pi_k \exp(-x') = 1 - 2 \exp(-x').$$

Combining this bound with (8.9) and (8.10) completes the proof.  $\square$

## 8.2 Proof of Theorem 6.2

The following inequality will be useful.

**Lemma 8.2** (Projection matrices). *Let  $A, B$  be two squared matrices of size  $n$  with  $A^T = A = A^2$  and  $B^T = B = B^2$ . Then*

$$|\text{Tr}(A - B)| \leq \|A - B\|_F^2. \quad (8.12)$$

*Proof.* Without loss of generality, assume that  $\text{Tr} A \geq \text{Tr} B$ . As  $\|A - B\|_F^2 = \|A\|_F^2 + \|B\|_F^2 - 2\text{Tr}(AB)$  and  $\|A\|_F^2 = \text{Tr} A$ , (8.12) is equivalent to  $2\text{Tr}(AB) \leq 2\text{Tr}(B)$ . Notice that for projection matrices,  $\text{Tr}(AB) = \|AB\|_F^2 \leq \|A\|_2^2 \|B\|_F^2 \leq \|B\|_F^2 = \text{Tr}(B)$  and the proof is complete.  $\square$

*Proof of Theorem 6.2.* Let  $\hat{\boldsymbol{\theta}} = \hat{\boldsymbol{\theta}}_{\hat{\sigma}}$  for notational simplicity. Similarly to the proof of Theorem 2.1, inequality (8.3) with  $F = W_{\text{pen}}$  and  $\boldsymbol{\theta} = \mathbf{e}_q$  implies

$$\|\hat{\boldsymbol{\mu}}_{\hat{\boldsymbol{\theta}}} - \mathbf{f}\|_2^2 \leq \min_{q=1,\dots,M} \|\hat{\boldsymbol{\mu}}_q - \mathbf{f}\|_2^2 + \max_{j,k=1,\dots,M} \zeta_{j,k},$$

where

$$\begin{aligned}\zeta_{j,k} &= \boldsymbol{\xi}^T Q_{j,k} \boldsymbol{\xi} - \mathbb{E}[\boldsymbol{\xi}^T Q_{j,k} \boldsymbol{\xi}] + \boldsymbol{\xi}^T \mathbf{v}_{j,k} - \frac{1}{2} \|(A_k - A_j) \mathbf{f} + \mathbf{b}_k - \mathbf{b}_j\|_2^2 \\ &\quad + 2(\hat{\sigma}^2 - \sigma^2) \text{Tr}(A_j - A_k) - \frac{\sigma^2}{2} \|A_k - A_j\|_F^2,\end{aligned}$$

the matrices  $Q_{j,k}$  and the vectors  $\mathbf{v}_{j,k}$  are defined in (8.4) and (8.5). Let  $j, k \in \{1, \dots, M\}$ . The assumption on  $\hat{\sigma}^2$  and (8.12) yield that on an event  $\Omega_0$  of probability greater than  $1 - \delta$ ,

$$2|(\hat{\sigma}^2 - \sigma^2) \text{Tr}(A_j - A_k)| \leq \frac{\sigma^2}{4} \|A_j - A_k\|_F^2.$$

On the event  $\Omega_0$ ,

$$\begin{aligned}\zeta_{j,k} &\leq \boldsymbol{\xi}^T Q_{j,k} \boldsymbol{\xi} - \mathbb{E}[\boldsymbol{\xi}^T Q_{j,k} \boldsymbol{\xi}] + \boldsymbol{\xi}^T \mathbf{v}_{j,k} - \frac{1}{2} \|(A_k - A_j) \mathbf{f} + \mathbf{b}_k - \mathbf{b}_j\|_2^2 \\ &\quad - \frac{\sigma^2}{4} \|A_k - A_j\|_F^2.\end{aligned}$$

We apply (3.4) to the matrix  $Q_{j,k}$  and (3.3) to the vector  $\mathbf{v}_{j,k}$ . For all  $x > 0$ , it yields that on an event  $\Omega_{j,k}(x)$  of probability greater than  $1 - 2\exp(-x)$ ,

$$\begin{aligned}\boldsymbol{\xi}^T Q_{j,k} \boldsymbol{\xi} - \mathbb{E}[\boldsymbol{\xi}^T Q_{j,k} \boldsymbol{\xi}] &\leq \sigma^2(12x + 6 \|A_k - A_j\|_F \sqrt{x}), \\ &\leq 48\sigma^2 x + \frac{\sigma^2}{4} \|A_k - A_j\|_F^2,\end{aligned}$$

and (8.8) hold. On the event  $\Omega_0 \cap \Omega_{j,k}(x)$ , we have  $\zeta_{j,k} \leq 64\sigma^2 x$ . Using the union bound, the probability of the event  $\Omega_0 \cap (\cap_{j,k=1,\dots,M} \Omega_{j,k}(x))$  is at least

$$1 - \delta - 2M^2 \exp(-x).$$

Finally, on this event  $\max_{j,k=1,\dots,M} \zeta_{j,k} \leq 64\sigma^2 x$ . Setting  $x' = x - 2\log(M)$  completes the proof.  $\square$

### 8.3 Lower bound

*Proof of Proposition 2.1.* The lower bounds of [37, Theorem 5.4] are stated in expectation, but inspection of the proof of [37, Theorem 5.3 with  $S = 1$ ,  $\delta = \infty$  and  $R = \log(1 + eM)$ ] reveals that the lower bound holds also in probability since it is an application of [43, Theorem 2.7]. This result yields that there exist absolute constants  $p, c, C > 0$  and  $\mathbf{f}_1, \dots, \mathbf{f}_M \in \mathbf{R}^n$  such that for any estimator  $\hat{\boldsymbol{\mu}}$ ,

$$\sup_{j=1,\dots,M} \mathbb{P}_{\mathbf{f}_j}(\Omega_j) \geq p, \quad \Omega_j := \left\{ \|\hat{\boldsymbol{\mu}} - \mathbf{f}_j\|_2^2 \geq c\sigma^2 \log(M) \right\},$$

provided that  $\log(M) \leq cn$  and  $n, M > C$ . Set  $\mathbf{b}_j = \mathbf{f}_j$  for all  $j = 1, \dots, M$ . This lower bound implies that for any estimator  $\hat{\boldsymbol{\mu}}$ ,

$$\sup_{\mathbf{f} \in \mathbf{R}^n} \mathbb{P}_{\mathbf{f}} \left( \|\hat{\boldsymbol{\mu}} - \mathbf{f}\|_2^2 - \min_{k=1, \dots, M} \|\mathbf{b}_k - \mathbf{f}\|_2^2 \geq c\sigma^2 \log(M) \right) \geq p.$$

For all  $j = 1, \dots, M$ , let  $A_j = (1/\|\mathbf{f}_j\|_2^2)\mathbf{f}_j\mathbf{f}_j^T$  so that  $A_j$  is the orthogonal projection on the linear span of  $\mathbf{f}_j$ . The orthoprojector  $A_j$  has rank one so under  $\mathbb{P}_{\mathbf{f}_j}$ ,  $\|A_j\mathbf{y} - \mathbf{f}_j\|_2^2/\sigma^2$  is a  $\chi^2$  random variable with one degree of freedom. Let  $\Omega'_j$  be the event  $\{\|A_j\mathbf{y} - \mathbf{f}_j\|_2^2 \leq c\sigma^2 \log(M)/2\}$  and let  $\bar{\Omega}'_j$  be its complementary event. A two sided bound on the Gaussian tail implies that  $\mathbb{P}_{\mathbf{f}_j}(\bar{\Omega}'_j) \leq 2/(M^{c/4})$ , which is smaller than  $p/2$  if  $M$  is larger than some absolute constant, so that we have  $\mathbb{P}_{\mathbf{f}_j}(\bar{\Omega}_j \cup \bar{\Omega}'_j) \leq 1 - p + p/2$  where  $\bar{\Omega}_j$  is the complementary of  $\Omega_j$ , which implies  $\mathbb{P}_{\mathbf{f}_j}(\Omega_j \cap \Omega'_j) \geq p/2$ . Thus, for any estimator  $\hat{\boldsymbol{\mu}}$  and  $M$  large enough,

$$\sup_{\mathbf{f} \in \{\mathbf{f}_1, \dots, \mathbf{f}_M\}} \mathbb{P}_{\mathbf{f}} \left( \|\hat{\boldsymbol{\mu}} - \mathbf{f}\|_2^2 - \min_{k=1, \dots, M} \|A_k\mathbf{y} - \mathbf{f}\|_2^2 \geq c\sigma^2 \log(M)/2 \right) \geq p/2 =: p^*.$$

□

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# Supplement: additional proofs

## A Proof of Proposition 3.1

*Proof of Proposition 3.1.* Let  $a \in (0, 1)$ . By definition of  $\hat{J}$ , we have for all  $k = 1, \dots, M$ ,

$$\begin{aligned} \|\hat{\boldsymbol{\mu}}_j - \mathbf{f}\|_2^2 &\leq \|\hat{\boldsymbol{\mu}}_k - \mathbf{f}\|_2^2 + \Delta_{jk} - \frac{a}{2} \|\hat{\boldsymbol{\mu}}_j - \hat{\boldsymbol{\mu}}_k\|_2^2 + \frac{a}{2} \|\hat{\boldsymbol{\mu}}_j - \hat{\boldsymbol{\mu}}_k\|_2^2, \\ &\leq \|\hat{\boldsymbol{\mu}}_k - \mathbf{f}\|_2^2 + \frac{1}{a} \max_{j,k=1,\dots,M} \left( a\Delta_{jk} - \frac{1}{2} \|a\hat{\boldsymbol{\mu}}_j - a\hat{\boldsymbol{\mu}}_k\|_2^2 \right) \\ &\quad + a(\|\hat{\boldsymbol{\mu}}_j - \mathbf{f}\|_2^2 + \|\mathbf{f} - \hat{\boldsymbol{\mu}}_k\|_2^2). \end{aligned}$$

By rearranging, we have almost surely

$$\|\hat{\boldsymbol{\mu}}_j - \mathbf{f}\|_2^2 \leq \frac{1+a}{1-a} \min_{k=1,\dots,M} \|\hat{\boldsymbol{\mu}}_k - \mathbf{f}\|_2^2 + \frac{\Xi}{a(1-a)},$$

$$\text{where } \Xi := \max_{j,k=1,\dots,M} \left( 2\boldsymbol{\xi}^T(\hat{\boldsymbol{\mu}}'_j - \hat{\boldsymbol{\mu}}'_k) - 2\sigma^2 \text{Tr}(A'_j - A'_k) - \frac{1}{2} \|\hat{\boldsymbol{\mu}}'_j - \hat{\boldsymbol{\mu}}'_k\|_2^2 \right),$$

and for all  $j = 1, \dots, M$ ,  $\hat{\boldsymbol{\mu}}'_j := a\hat{\boldsymbol{\mu}}_j = A'_j \mathbf{y} + \mathbf{b}'_j$ ,  $A'_j := aA_j$ ,  $\mathbf{b}'_j := a\mathbf{b}_j$ , and  $\|A'_j\|_2 \leq 1$ . It is shown in the proof of Theorem 2.1 that with probability greater than  $1 - 2\exp(-x)$ ,  $\Xi \leq 46\sigma^2(x + 2\log M)$ .

Set  $\epsilon = 3a$  and choose the absolute constant  $c > 0$  such that for all  $\epsilon < c$ ,  $(1+a)/(1-a) \leq 1 + \epsilon$  and  $1/(1-a) \leq 2$ . Set  $C = 276$  to complete the proof.  $\square$

## B Smoothness adaptation

*Proof of Proposition 7.1.* Because the ellipsoids are ordered, if  $\mathbf{f} \in \Theta(\beta, L)$  then

$$\mathbb{E}\|\mathbf{f} - \tilde{\boldsymbol{\mu}}\|_2^2 \leq \min_{j:\beta_j \leq \beta} \mathbb{E}\|\mathbf{f} - A_{\beta_j} \mathbf{y}\|_2^2 + 92\sigma^2 \log M \leq \min_{j:\beta_j \leq \beta} C^* n^{\frac{1}{2\beta_j+1}} (1 + o(1)).$$

If  $\beta \in [\beta_j, \beta_{j+1})$  for some  $j$ , then  $\beta_{j+1} - \beta_j = \beta_j / (\log(n) \log \log n)$  and simple algebra yields

$$n^{\frac{1}{2\beta_j+1} - \frac{1}{2\beta+1}} \leq n^{\frac{2\beta_{j+1}-2\beta_j}{(2\beta+1)(2\beta_j+1)}} = n^{\frac{2\beta_j}{(2\beta+1)(2\beta_j+1)\log(n)\log \log n}} \leq n^{\frac{1}{(2\beta+1)\log(n)\log \log n}} \leq e^{\frac{1}{3\log \log n}},$$

where we used that  $\beta \geq 1$  for the last inequality.

Now assume that  $\beta \geq \beta_M$ . Let  $\epsilon_n = 1/(\log(n) \log \log n)$ , and

$$c = 120 \log(1 + \epsilon_3)/\epsilon_3.$$

By definition of  $M$ ,

$$\beta_M = e^{M \log\left(1 + \frac{1}{\log(n) \log \log n}\right)} \geq e^{120 \log \log(n) \frac{\log(1+\epsilon_n)}{\epsilon_n}} \geq e^{c \log \log(n)} = \log(n)^c,$$

since the function  $t \rightarrow \log(1+t)/t$  is decreasing and  $n \geq 3$ . A numerical approximation gives  $c \geq 1.01$ . Thus,

$$n^{\frac{1}{2\beta_M+1}} n^{\frac{-1}{2\beta+1}} \leq n^{\frac{1}{2\beta_M+1}} \leq e^{\frac{\log n}{2\beta_M}} \leq e^{\frac{1}{2 \log(n)^{c-1}}}.$$

In summary we have proved that  $\min_{j: \beta_j \leq \beta} n^{\frac{1}{2\beta_j+1}} \leq n^{\frac{1}{2\beta+1}} (1 + o(1))$ , thus

$$\sup_{\mathbf{f} \in \Theta(\beta, L)} \mathbb{E} \|\mathbf{f} - \tilde{\boldsymbol{\mu}}\|_2^2 \leq C^* n^{\frac{1}{2\beta+1}} (1 + o(1)).$$

□

## C Convex aggregation

**Lemma C.1** (Maurey argument). *Let  $m$  and  $\Lambda_m^M$  be defined in (7.2) and (7.3). Let  $Q(\boldsymbol{\theta}) = \boldsymbol{\theta}^T \Sigma \boldsymbol{\theta} + \mathbf{v}^T \boldsymbol{\theta} + a$  for some semi-definite matrix  $\Sigma$ ,  $\mathbf{v} \in \mathbf{R}^M$  and  $a \in \mathbf{R}$ . Then*

$$\min_{\boldsymbol{\theta} \in \Lambda_m^M} Q(\boldsymbol{\theta}) \leq \min_{\boldsymbol{\theta} \in \Lambda^M} Q(\boldsymbol{\theta}) + \frac{4 \max_{j=1, \dots, M} \Sigma_{jj}}{m}. \quad (\text{C.1})$$

*Proof of Lemma C.1.* Let  $\boldsymbol{\theta}^* \in \Lambda^M \in \text{argmin}_{\boldsymbol{\theta} \in \Lambda^M} Q(\boldsymbol{\theta})$ . Let  $\eta$  be a random variable valued in  $\{\mathbf{e}_1, \dots, \mathbf{e}_M\}$  such that  $\mathbb{P}(\eta = \mathbf{e}_j) = \theta_j^*$  for all  $j = 1, \dots, M$ , and let  $\eta_1, \dots, \eta_m$  be  $m$  i.i.d. copies of  $\eta$ . The random variable  $\bar{\eta} = \frac{1}{m} \sum_{q=1}^m \eta_q$  is valued in  $\Lambda_m^M$  and  $\mathbb{E} \bar{\eta} = \boldsymbol{\theta}^*$ . A bias variance decomposition and the independence of  $\eta_1, \dots, \eta_m$  yield

$$\mathbb{E} Q(\bar{\eta}) = Q(\boldsymbol{\theta}^*) + \frac{\mathbb{E}[(\eta_1 - \boldsymbol{\theta}^*)^T \Sigma (\eta_1 - \boldsymbol{\theta}^*)]}{m}.$$

Using the triangle inequality,  $\mathbb{E}[(\eta_1 - \boldsymbol{\theta}^*)^T \Sigma (\eta_1 - \boldsymbol{\theta}^*)] \leq 2(\boldsymbol{\theta}^*)^T \Sigma \boldsymbol{\theta}^* + 2\mathbb{E}[\eta_1^T \Sigma \eta_1] \leq 4 \max_{j=1, \dots, M} \Sigma_{jj}$ . Since  $\bar{\eta}$  is valued in  $\Lambda_m^M$ ,  $\min_{\boldsymbol{\theta} \in \Lambda_m^M} Q(\boldsymbol{\theta}) \leq \mathbb{E} Q(\bar{\eta})$  and the proof is complete. □

*Proof of (7.5) of Proposition 7.2.* The condition on  $M, n$  implies that  $m \geq 1$  where  $m$  is defined in (7.2). Let  $C > 0$  be an absolute constant whose value may change from line to line. Applying Theorem 2.1 yields that on an event of probability greater than  $1 - 2\exp(-x)$ ,

$$\frac{1}{n} \|\hat{\boldsymbol{\mu}}_{\Lambda_m^M} - \mathbf{f}\|_2^2 \leq \min_{\boldsymbol{\theta} \in \Lambda_m^M} \frac{1}{n} \|\hat{\boldsymbol{\mu}}_{\boldsymbol{\theta}} - \mathbf{f}\|_2^2 + \frac{C\sigma^2(\log(|\Lambda_m^M|) + x)}{n}. \quad (\text{C.2})$$

By [29, page 8] we have

$$\log |\Lambda_m^M| \leq m \log \frac{2eM}{m}.$$

We use (C.1) with  $Q(\boldsymbol{\theta}) = \|\hat{\boldsymbol{\mu}}_{\boldsymbol{\theta}} - \mathbf{f}\|_2^2$  to get

$$\min_{\boldsymbol{\theta} \in \Lambda_m^M} \frac{1}{n} \|\hat{\boldsymbol{\mu}}_{\boldsymbol{\theta}} - \mathbf{f}\|_2^2 \leq \min_{\boldsymbol{\theta} \in \Lambda^M} \frac{1}{n} \|\hat{\boldsymbol{\mu}}_{\boldsymbol{\theta}} - \mathbf{f}\|_2^2 + \frac{4}{nm} \max_{j=1, \dots, M} \|\hat{\boldsymbol{\mu}}_j\|_2^2.$$

We have  $(1/n) \max_{j=1, \dots, M} \|\hat{\boldsymbol{\mu}}_j\|_2^2 \leq C(\|\boldsymbol{\xi}\|_2^2/n + R^2) \leq C(\sigma^2(2+3x) + R^2)$  on an event of probability at least  $1 - \exp(-x)$ , where for the second inequality we used (3.4) with  $B = I_{n \times n}$ . Thus, with probability greater than  $1 - e^{-x}$ ,

$$\min_{\boldsymbol{\theta} \in \Lambda_m^M} \frac{1}{n} \|\hat{\boldsymbol{\mu}}_{\boldsymbol{\theta}} - \mathbf{f}\|_2^2 \leq \min_{\boldsymbol{\theta} \in \Lambda^M} \frac{1}{n} \|\hat{\boldsymbol{\mu}}_{\boldsymbol{\theta}} - \mathbf{f}\|_2^2 + \frac{C(\sigma^2(2+3x) + R^2)}{m}. \quad (\text{C.3})$$

Simple algebra yields that

$$\frac{1}{m} \leq C \sqrt{\frac{\log(1 + M/\sqrt{n})}{n}}, \quad \frac{m \log(2eM/m)}{n} \leq C \sqrt{\frac{\log(1 + M/\sqrt{n})}{n}}. \quad (\text{C.4})$$

Combining (C.2), (C.3) and (C.4) with the union bound completes the proof.  $\square$

*Proof of (7.4) of Proposition 7.2.* Let  $\boldsymbol{\theta} \in \Lambda^M$ . By definition of  $\hat{\boldsymbol{\theta}}_C$ ,  $C_p(\hat{\boldsymbol{\theta}}) \leq C_p(\boldsymbol{\theta})$ . This can be rewritten

$$\|\hat{\boldsymbol{\mu}}_{\hat{\boldsymbol{\theta}}_C} - \mathbf{f}\|_2^2 \leq \|\hat{\boldsymbol{\mu}}_{\hat{\boldsymbol{\theta}}} - \mathbf{f}\|_2^2 + 2\boldsymbol{\xi}^T(\hat{\boldsymbol{\mu}}_{\hat{\boldsymbol{\theta}}} - \hat{\boldsymbol{\mu}}_{\boldsymbol{\theta}}).$$

The function  $(\boldsymbol{\theta}', \boldsymbol{\theta}) \rightarrow 2\boldsymbol{\xi}^T(\hat{\boldsymbol{\mu}}_{\hat{\boldsymbol{\theta}}} - \hat{\boldsymbol{\mu}}_{\boldsymbol{\theta}})$  is bilinear, thus it is maximized at vertices, and

$$2\boldsymbol{\xi}^T(\hat{\boldsymbol{\mu}}_{\hat{\boldsymbol{\theta}}} - \hat{\boldsymbol{\mu}}_{\boldsymbol{\theta}}) \leq \max_{j,k=1, \dots, M} 2\boldsymbol{\xi}^T(\hat{\boldsymbol{\mu}}_k - \hat{\boldsymbol{\mu}}_j) = \max_{j,k=1, \dots, M} \Delta_{jk},$$

where  $\Delta_{jk}$  is defined in (3.2). Fix some pair  $(j, k)$ . Let  $B = A_j - A_k$  and  $\mathbf{b} = (A_j - A_k)\mathbf{f} + \mathbf{b}_j - \mathbf{b}_k$ . We have  $\|B\|_2 \leq 2$ ,  $\|B\|_F \leq \|B\|_2 \|I_{n \times n}\|_F \leq 2\sqrt{n}$  and  $\|\mathbf{b}\|_2 \leq 4R\sqrt{n}$ . We apply (3.4) to the matrix  $B$  and (3.3) to the vector  $\mathbf{b}$ , which yields that with probability greater than  $1 - 2\exp(-x)$ ,

$$\Delta_{jk} \leq 8(\sigma^2 + \sigma R\sqrt{2})\sqrt{nx} + 8\sigma^2 x.$$

The union bound over all pairs  $j, k = 1, \dots, M$  completes the proof.  $\square$

## D Sparsity oracle inequalities

### D.1 Concentration inequalities for subgaussian vectors

A direct consequence of assumption (7.8) on the random vector  $\boldsymbol{\xi}$  is the following Hoeffding-type concentration inequality:

$$\mathbb{P}(\alpha^T \boldsymbol{\xi} > K\|\alpha\|_2 \sqrt{2x}) \leq \exp(-x). \quad (\text{D.1})$$

The following concentration inequality was proven in [25].

**Proposition D.1** (One sided concentration [25]). *Let  $\boldsymbol{\xi}$  be a random vector in  $\mathbf{R}^n$  satisfying (7.8) for some  $K > 0$ . Let  $A$  be a real  $n \times n$  positive semi-definite symmetric matrix. Then for all  $x > 0$ , with probability greater than  $1 - \exp(-x)$ ,*

$$\boldsymbol{\xi}^T A \boldsymbol{\xi} \leq K^2 (\text{Tr} A + 2\|A\|_F \sqrt{x} + 2\|A\|_2 x). \quad (\text{D.2})$$

This result is remarkable as it holds with the same constants as in the Gaussian case (3.4), under the weak assumption (7.8).

**Corollary D.1** (Corollary of Proposition D.1 for any real matrix  $A$ ). *Under (7.8) and for any real matrix  $A$ , with probability greater than  $1 - \exp(-x)$ , the following holds:*

$$\boldsymbol{\xi}^T A \boldsymbol{\xi} \leq K^2 (\|A\|_1 + 2\|A\|_F \sqrt{x} + 2\|A\|_2 x). \quad (\text{D.3})$$

*Proof.* To see this, let  $A_s := \frac{1}{2}(A + A^T)$  and let  $|A_s| := \sqrt{A_s^2}$ , the square root of the positive semi-definite symmetric matrix  $A_s^2$ . By definition of  $|A_s|$  and the triangle inequality,

$$\begin{aligned} \boldsymbol{\xi}^T A \boldsymbol{\xi} &= \boldsymbol{\xi}^T A_s \boldsymbol{\xi} \leq \boldsymbol{\xi}^T |A_s| \boldsymbol{\xi}, & \text{Tr}(|A_s|) &= \|A_s\|_1 \leq \|A\|_1, \\ \| |A_s| \|_2 &= \|A_s\|_2 \leq \|A\|_2, & \| |A_s| \|_F &= \|A_s\|_F \leq \|A\|_F. \end{aligned}$$

Thus applying (D.2) to the matrix  $|A_s|$  proves (D.3).  $\square$

In [25], the authors prove the following oracle inequality for the Least Squares estimator  $\hat{\boldsymbol{\mu}}_V^{LS}$  on a  $d$ -dimensional linear subspace  $V$  of  $\mathbf{R}^n$ . The Least Squares estimator  $\hat{\boldsymbol{\mu}}_V^{LS}$  is defined as the orthogonal projection of  $\mathbf{y}$  on the linear subspace  $V$ .

**Lemma D.1** ([25]). *Under (7.8), with probability greater than  $1 - \exp(-x)$ :*

$$\begin{aligned} \|\hat{\boldsymbol{\mu}}_V^{LS} - \mathbf{f}\|_2^2 &\leq \min_{\mu \in V} \|\mu - \mathbf{f}\|_2^2 + K^2(d + 2\sqrt{dx} + 2x), \\ &\leq \min_{\mu \in V} \|\mu - \mathbf{f}\|_2^2 + K^2(2d + 3x). \end{aligned} \quad (\text{D.4})$$

## D.2 Preliminary result

Under the assumption (7.8), the authors of [25] proved the concentration inequality (D.2) and we use this concentration result to prove the following oracle inequality for aggregation of Least Squares estimators. Given an estimator  $\hat{K}^2$ , define for any  $\boldsymbol{\theta} \in \Lambda^M$

$$U(\boldsymbol{\theta}) = \|\hat{\boldsymbol{\mu}}_{\boldsymbol{\theta}}\|_2^2 - 2\mathbf{y}^T \hat{\boldsymbol{\mu}}_{\boldsymbol{\theta}} + \frac{1}{2} \text{pen}(\boldsymbol{\theta}) + 32\hat{K}^2 \sum_{j=1}^M \theta_j \log \frac{1}{\pi_j},$$

where  $\text{pen}(\cdot)$  is the penalty (2.3). We consider the estimator  $\hat{\boldsymbol{\mu}}_{\hat{\boldsymbol{\theta}}}$  of  $\mathbf{f}$  where

$$\hat{\boldsymbol{\theta}} \in \underset{\boldsymbol{\theta} \in \Lambda^M}{\text{argmin}} U(\boldsymbol{\theta}). \quad (\text{D.5})$$

The function  $U$  is equal to the sum of  $H_{\text{pen}}$  (2.2) and some linear function of  $\boldsymbol{\theta}$ . Thus  $U$  is also convex.

**Proposition D.2.** *Let  $K > 0$  be the smallest positive number such that the random vector  $\boldsymbol{\xi}$  satisfies (7.8). For all  $j = 1, \dots, M$ , let  $\mathbf{b}_j \in \mathbf{R}^n$  and let  $A_j$  be a square matrix of size  $n$  that satisfies  $A_j = A_j^T = A_j^2$ . Let  $(\pi_1, \dots, \pi_M) \in \Lambda^M$  such that for all  $j = 1, \dots, M$ ,  $\text{Tr}(A_j) \leq \log(\pi_j^{-1})$ . Let  $\hat{K} > 0$  be a given estimator and let  $\hat{\boldsymbol{\theta}}$  be defined in (D.5). Let  $\delta := \mathbb{P}(\hat{K}^2 < K^2)$ . Then for all  $x > 0$ , with probability greater than  $1 - \delta - 2\exp(-x)$ ,*

$$\|\hat{\boldsymbol{\mu}}_{\hat{\boldsymbol{\theta}}} - \mathbf{f}\|_2^2 \leq \min_{j=1, \dots, M} \left( \|\hat{\boldsymbol{\mu}}_j - \mathbf{f}\|_2^2 + 64\hat{K}^2 \log \frac{1}{\pi_j} \right) + 28K^2x.$$

Proposition D.2 is proved below. Compared to (5.2), this oracle inequality holds for orthogonal projectors under the constraint  $\text{Tr}(A_j) \leq \log(\pi_j^{-1})$  for all  $j = 1, \dots, M$ . However, this oracle inequality presents some advantages.

First, it holds under (7.8) which is weaker than the Gaussian assumption of Theorem 5.1 since the noise coordinates do not need to be independent. Second, the quantity  $K^4/\sigma^2$  that appears in (6.4) is not present here, which is possible thanks to the constraint  $\text{Tr}(A_j) \leq \log(\pi_j^{-1})$ . This repairs the drawback of the right hand side of (6.4) which may be large if the noise random variables have a pathologically small variance compared to their subgaussian norm. Finally, one does not need to know the variance of the noise in order to compute the proposed estimator; its construction only relies on  $\hat{K}$  which can be any estimate that *upper bounds* the subgaussian norm of the random vector  $\xi$ . For instance, assume that  $\xi$  is zero-mean Gaussian with covariance matrix  $\sigma^2 I_{n \times n}$ , and assume that an estimator  $\hat{\sigma}^2$  of  $\sigma^2$  is accessible, and that this estimator has bounded bias. Let  $\gamma > 1$  and  $\epsilon = \mathbb{P}(\hat{\sigma}^2 < \sigma^2/\gamma)$ . The quantity  $\epsilon$  is likely to be small if  $\hat{\sigma}^2$  has a bounded bias and  $\gamma$  is large enough. Then one can use the upper bound  $\hat{K}^2 = \gamma \hat{\sigma}^2$  in Proposition D.2, which yields that with probability greater than  $1 - 3\epsilon$ ,

$$\|\hat{\mu}_{\hat{\theta}} - \mathbf{f}\|_2^2 \leq \min_{j=1, \dots, M} \left( \|\hat{\mu}_j - \mathbf{f}\|_2^2 + 64\gamma \hat{\sigma}^2 \log \frac{1}{\pi_j} \right) + 28\sigma^2 \log(1/\epsilon).$$

Thus,  $\gamma$  is used to perform a trade-off between the probability estimate and the remainder term of the oracle inequality. By using an upper bound for  $\hat{K}^2$  in Proposition D.2 the oracle inequality holds with slightly worse constants but with high probability.

*Proof of Proposition D.2.* Let  $\hat{\beta} = 32\hat{K}^2$ . Let  $q = 1, \dots, M$  be a deterministic integer. Inequality (8.3) with  $F = U$  can be rewritten as

$$\|\hat{\mu}_{\hat{\theta}} - \mathbf{f}\|_2^2 \leq \|\hat{\mu}_q - \mathbf{f}\|_2^2 + 2\hat{\beta} \log \frac{1}{\pi_q} + z(q, \hat{\theta})$$

where

$$z(q, \hat{\theta}) := 2\xi^T(\hat{\mu}_{\hat{\theta}} - \hat{\mu}_q) - \frac{1}{2} \sum_{k=1}^M \hat{\theta}_k \|\hat{\mu}_k - \hat{\mu}_q\|_2^2 - \hat{\beta} \log \frac{1}{\pi_q} - \hat{\beta} \sum_{k=1}^M \hat{\theta}_k \log \frac{1}{\pi_k}.$$

The function  $z(q, \cdot)$  is affine in its second argument. Thus it is maximized at a vertex of  $\Lambda^M$ , and

$$z(q, \hat{\theta}) \leq \max_{\theta \in \Lambda^M} z(q, \theta) = \max_{k=1, \dots, M} z(q, \mathbf{e}_k) \leq \max_{j, k=1, \dots, M} z(j, \mathbf{e}_k).$$

As it holds for all deterministic  $q = 1, \dots, M$ , we proved that

$$\|\hat{\mu}_{\hat{\theta}} - \mathbf{f}\|_2^2 \leq \min_{q=1, \dots, M} \left( \|\hat{\mu}_q - \mathbf{f}\|_2^2 + 2\hat{\beta} \log \frac{1}{\pi_q} \right) + \max_{j, k=1, \dots, M} \zeta_{jk},$$

where

$$\zeta_{jk} := z(j, \mathbf{e}_k) = 2\boldsymbol{\xi}^T(\hat{\boldsymbol{\mu}}_k - \hat{\boldsymbol{\mu}}_j) - \hat{\beta} \log \frac{1}{\pi_j \pi_k} - \frac{1}{2} \|\hat{\boldsymbol{\mu}}_k - \hat{\boldsymbol{\mu}}_j\|_2^2.$$

Let  $B_{jk} = A_k - A_j$ , and note that  $\|B_{jk}\|_2 \leq 2$  because  $A_k$  and  $A_j$  are orthogonal projectors. Using  $\hat{\boldsymbol{\mu}}_k - \hat{\boldsymbol{\mu}}_j = B_{jk}\boldsymbol{\xi} + (B_{jk}\mathbf{f} + \mathbf{b}_k - \mathbf{b}_j)$ , we get

$$\zeta_{jk} = 2\boldsymbol{\xi}^T(A_k - A_j)\boldsymbol{\xi} + \boldsymbol{\xi}^T\alpha_{jk} - \frac{1}{2}\|B_{jk}\mathbf{f} + \mathbf{b}_k - \mathbf{b}_j\|_2^2 - \frac{1}{2}\|B_{jk}\boldsymbol{\xi}\|_2^2 - \hat{\beta} \log \frac{1}{\pi_j \pi_k},$$

where  $\alpha_{jk} := 2(I_{n \times n} - \frac{1}{2}B_{jk}^T)(B_{jk}\mathbf{f} + \mathbf{b}_k - \mathbf{b}_j)$ . The vector  $\alpha_{jk}$  satisfies

$$\|\alpha_{jk}\|_2 \leq 2(1 + \frac{1}{2}\|B_{jk}\|_2)\|B_{jk}\mathbf{f} + \mathbf{b}_k - \mathbf{b}_j\|_2 \leq 4\|B_{jk}\mathbf{f} + \mathbf{b}_k - \mathbf{b}_j\|_2.$$

We also have  $-\|B_{jk}\boldsymbol{\xi}\|_2^2 \leq 0$  almost surely.

Let  $x > 0$ . We now apply the concentration inequality (D.3) to the matrix  $2B_{jk}$  and the Hoeffding-type inequality (D.1) to the vector  $\alpha_{jk}$ . Using the union bound, the following holds with probability greater than  $1 - 2\exp(-x)$ :

$$\begin{aligned} \zeta_{jk} \leq & K^2(2\|B_{jk}\|_1 + 4\|B_{jk}\|_2 x + 4\|B_{jk}\|_F \sqrt{x}) \\ & + 2K(1 + \frac{1}{2}\|B_{jk}\|_2)\|B_{jk}\mathbf{f} + \mathbf{b}_k - \mathbf{b}_j\|_2 \sqrt{2x} - \frac{1}{2}\|B_{jk}\mathbf{f} + \mathbf{b}_k - \mathbf{b}_j\|_2^2 \\ & - \hat{\beta} \log \frac{1}{\pi_j \pi_k}. \end{aligned}$$

We upper bound the first line of the RHS of the previous display. By the triangle inequality, and the assumption  $\text{Tr}(A_j) \leq \log(\pi_j^{-1})$ , we have  $\|B_{jk}\|_1 \leq \text{Tr}(A_j + A_k) \leq \log((\pi_j \pi_k)^{-1})$ . Using simple inequalities,

$$\|B_{jk}\|_F \sqrt{x} \leq (\|A_j\|_F + \|A_k\|_F) \sqrt{x} \leq (\|A_j\|_F^2 + \|A_k\|_F^2 + 2x)/2 \leq \frac{1}{2} \log \frac{1}{\pi_j \pi_k} + x.$$

Thus,  $2\|B_{jk}\|_1 + 4\|B_{jk}\|_2 x + 4\|B_{jk}\|_F \sqrt{x} \leq K^2(12x + 4 \log \frac{1}{\pi_j \pi_k})$ .

Now we upper bound the second line. We apply the inequality  $st \leq \frac{s^2 + t^2}{2}$  with  $t = \|B_{jk}\mathbf{f} + \mathbf{b}_k - \mathbf{b}_j\|_2$  and  $s = 2K(1 + \frac{1}{2}\|B_{jk}\|_2)\sqrt{2x}$ :

$$\begin{aligned} & 2K(1 + \frac{1}{2}\|B_{jk}\|_2)\|B_{jk}\mathbf{f} + \mathbf{b}_k - \mathbf{b}_j\|_2 \sqrt{2x} - \frac{1}{2}\|B_{jk}\mathbf{f} + \mathbf{b}_k - \mathbf{b}_j\|_2^2 \\ & = st - \frac{t^2}{2} \leq \frac{s^2}{2} = 4K^2(1 + \frac{1}{2}\|B_{jk}\|_2)^2 x \leq 16K^2 x. \end{aligned}$$

For any  $x' > 0$ , let  $x_{jk} = x' + \frac{1}{\pi_j \pi_k}$ . By setting  $x = x_{jk}$ , the above displays yield the following bound on  $\zeta_{jk}$ , with probability greater than  $1 - 2\pi_j \pi_k \exp(-x')$ :

$$\zeta_{jk} \leq 28K^2 x_{jk} - (\hat{\beta} - 4K^2) \log \frac{1}{\pi_j \pi_k} = 28K^2 x' - (\hat{\beta} - 32K^2) \log \frac{1}{\pi_j \pi_k}.$$



Using a union bound, we obtain that on an event of probability greater than  $1 - \delta - 2 \sum_{j=1}^M \sum_{k=1}^M \pi_j \pi_k \exp(-x') = 1 - \delta - 2 \exp(-x')$ , we have  $\hat{\beta} \geq 32K^2$  and

$$\max_{j,k=1,\dots,M} \zeta_{jk} \leq 28K^2 x'.$$

□

### D.3 Sparsity pattern aggregation

We now combine (D.2) and (D.4) to prove Theorem 7.1.

*Proof of Theorem 7.1.* Given a subset  $J \subset \{1, \dots, p\}$ , the projection matrix  $A_J$  satisfies  $\text{Tr}(A_J) \leq |J| \leq \log(\pi_J^{-1})$  since the normalizing constant of the weights  $(\pi_j)_{J \subset \{1, \dots, p\}}$  is greater than 1 [38, Section 5.2.1]. The estimator  $\hat{\boldsymbol{\mu}}_J^{LS}$  satisfies the oracle inequality (D.4) with  $d \leq |J|$ , where  $|J|$  denotes the cardinal of  $J$  and  $d$  is the dimension of the linear span of the columns whose indices are in  $J$ .

Let  $\bar{\boldsymbol{\theta}} \in \mathbf{R}^p$  be a minimizer of the right hand side of (7.9) and let  $\bar{J} \subset \{1, \dots, p\}$  be the support of  $\bar{\boldsymbol{\theta}}$ , hence  $|\bar{\boldsymbol{\theta}}|_0 = |\bar{J}|$ . Since the RHS of (7.9) is random,  $\bar{\boldsymbol{\theta}}$  and its support are also random.

Let  $t > 0$ . For each support  $J \subset \{1, \dots, p\}$ , the oracle inequality (D.4) applied to  $x = t + \log(\pi_J^{-1})$  yields that with probability greater than  $1 - \pi_J \exp(-t)$ ,

$$\|\hat{\boldsymbol{\mu}}_J^{LS} - \mathbf{f}\|_2^2 \leq \|\mathbb{X}\bar{\boldsymbol{\theta}} - \mathbf{f}\|_2^2 + K^2 \left( 2|\bar{\boldsymbol{\theta}}|_0 + 3 \log \left( \frac{1}{\pi_J} \right) + 3t \right). \quad (\text{D.6})$$

With the union bound, (D.6) holds simultaneously for all  $J \subset \{1, \dots, p\}$  with probability greater than  $1 - \exp(-t) = 1 - \sum_{J \subset \{1, \dots, p\}} \pi_J \exp(-t)$ .

We apply the oracle inequality of Proposition D.2 and the oracle inequality (D.6) to  $\hat{\boldsymbol{\mu}}_J^{LS}$ . With the union bound, we have with probability greater than  $1 - \delta - 3 \exp(-t)$ :

$$\begin{aligned} \|\mathbb{X}\hat{\boldsymbol{\theta}}^{SPA} - \mathbf{f}\|_2^2 &\leq \|\hat{\boldsymbol{\mu}}_J^{LS} - \mathbf{f}\|_2^2 + 64\hat{K}^2 \log \frac{1}{\pi_{\bar{J}}} + 28K^2 t, \\ \|\hat{\boldsymbol{\mu}}_J^{LS} - \mathbf{f}\|_2^2 &\leq \|\mathbb{X}\bar{\boldsymbol{\theta}} - \mathbf{f}\|_2^2 + K^2 \left( 2|\bar{\boldsymbol{\theta}}|_0 + 3 \log \left( \frac{1}{\pi_{\bar{J}}} \right) + 3t \right), \end{aligned}$$

where  $A_{\bar{J}}$  is the projection matrix such that  $\hat{\boldsymbol{\mu}}_J^{LS} = A_{\bar{J}}\mathbf{y}$ . We now use the following bound from [38, Section 5.2.1]:

$$\log \frac{1}{\pi_{\bar{J}}} \leq 2|\bar{\boldsymbol{\theta}}|_0 \log \left( \frac{ep}{1 \vee |\bar{\boldsymbol{\theta}}|_0} \right) + \frac{1}{2}.$$

Summing the two oracle inequalities above and applying the upper bound on  $\log \frac{1}{\pi_j}$  completes the proof.  $\square$